Figure 1

Figure 2. The amino-acid sequence of the GST-GK fusion protein. The GST sequence was taken from GenBank entry U13852. Residue 229 of the fusion protein is the first residue of GK.

```
  1 MSPILGYWKI KGLVQPTRLL LEYLEEKYEE HLYERDEGDK WRNKKFELGL EFPNLPYYID
 61 GDVKLTQSMA IIRYIADKHN MLGGCPKERA EISMLEGAVL DIRYGVSRIA YSKDFETLKV
121 DFLSKLPEML KMFEDRLCHK TYLNGDHVTH PDFMLYDALD VVLYMDPMCL DAFPKLVCFK
181 KRIEAIPQID KYLKSSKYIA WPLQGWQATF GGGDHPPKSD LIEGRGIHMP RPRSQLPQPN
241 SQVEQILAEF QLQEEDLKKV MRRMQKEMDR GLRLETHEEA SVKMLPTYVR STPEGSEVGD
301 FLSLDLGGTN FRVMLVKVGE GEEGQWSVKT KHQMYSIPED AMTGTAEMLF DYISECISDF
361 LDKHQMKHKK LPLGFTFSFP VRHEDIDKGI LLNWTKGFKA SGAEGNNVVG LLRDAIKRRG
421 DFEMDVVAMV NDTVATMISC YYEDHQCEVG MIVGTGCNAC YMEEMQNVEL VEGDEGRMCV
481 NTEWGAFGDS GELDEFLLEY DRLVDESSAN PGQQLYEKLI GGKYMGELVR LVLLRLVDEN
541 LLFHGEASEQ LRTRGAFETR FVSQVESDTG DRKQIYNILS TLGLRPSTTD CDIVRRACES
601 VSTRAAHMCS AGLAGVINRM RESRSEDVMR ITVGVDGSVY KLHPSFKERF HASVRRLTPS
661 CEITFIESEE GSGRGAALVS AVACKKACML GQ
```
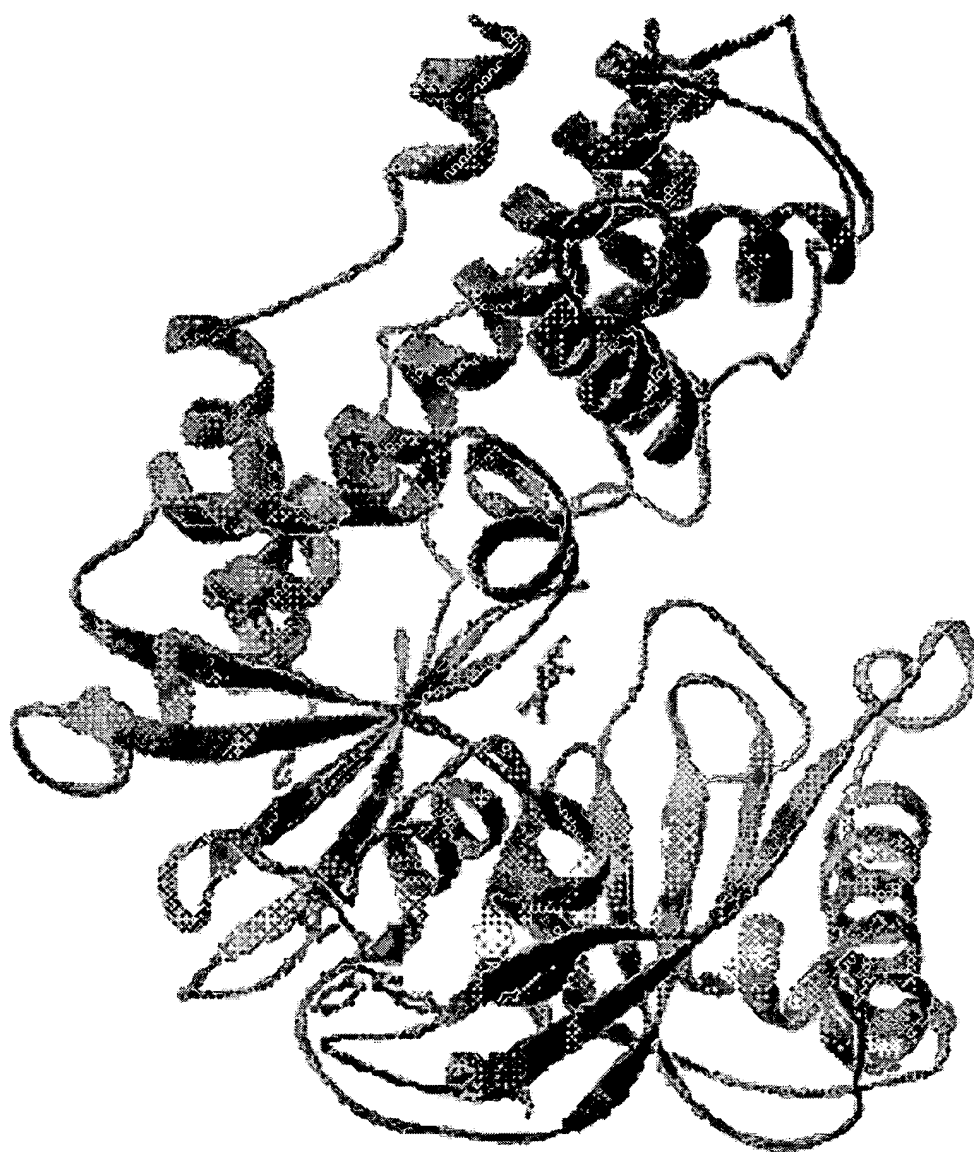
Figure 3

Figure 4   Sheet 1 of 62

Atom No.	Atom Type	A.A. Type	A.A. #	X	Y	Z	OCC	B
ATOM	1	CB	SER	8	-0.421	63.744	24.899	1.00	50.68
ATOM	2	OG	SER	8	-0.752	63.605	23.524	1.00	50.85
ATOM	3	C	SER	8	1.865	64.216	24.094	1.00	50.72
ATOM	4	O	SER	8	2.308	63.644	23.102	1.00	51.79
ATOM	5	N	SER	8	1.473	63.793	26.507	1.00	50.36
ATOM	6	CA	SER	8	1.057	63.446	25.120	1.00	50.55
ATOM	7	N	GLN	9	2.041	65.515	24.314	1.00	49.84
ATOM	8	CA	GLN	9	2.831	66.312	23.385	1.00	48.95
ATOM	9	CB	GLN	9	2.983	67.745	23.895	1.00	49.08
ATOM	10	CG	GLN	9	3.676	68.686	22.925	1.00	50.25
ATOM	11	CD	GLN	9	3.206	70.127	23.085	1.00	51.06
ATOM	12	OE1	GLN	9	2.037	70.433	22.846	1.00	51.38
ATOM	13	NE2	GLN	9	4.112	71.017	23.499	1.00	51.44
ATOM	14	C	GLN	9	4.190	65.633	23.294	1.00	48.56
ATOM	15	O	GLN	9	4.884	65.741	22.285	1.00	48.75
ATOM	16	N	VAL	10	4.560	64.926	24.361	1.00	47.77
ATOM	17	CA	VAL	10	5.823	64.198	24.392	1.00	46.87
ATOM	18	CB	VAL	10	6.293	63.902	25.842	1.00	46.39
ATOM	19	CG1	VAL	10	7.303	62.782	25.841	1.00	46.41
ATOM	20	CG2	VAL	10	6.952	65.135	26.436	1.00	46.79
ATOM	21	C	VAL	10	5.616	62.885	23.653	1.00	46.17
ATOM	22	O	VAL	10	6.521	62.384	22.991	1.00	46.18
ATOM	23	N	GLU	11	4.423	62.317	23.768	1.00	45.28
ATOM	24	CA	GLU	11	4.159	61.071	23.069	1.00	45.19
ATOM	25	CB	GLU	11	2.905	60.393	23.616	1.00	45.21
ATOM	26	CG	GLU	11	3.105	59.709	24.967	1.00	46.05
ATOM	27	CD	GLU	11	4.224	58.664	24.957	1.00	46.30
ATOM	28	OE1	GLU	11	4.350	57.918	23.948	1.00	46.28
ATOM	29	OE2	GLU	11	4.963	58.583	25.972	1.00	45.66
ATOM	30	C	GLU	11	4.002	61.345	21.580	1.00	44.48
ATOM	31	O	GLU	11	4.068	60.430	20.755	1.00	44.48
ATOM	32	N	GLN	12	3.807	62.614	21.239	1.00	43.86
ATOM	33	CA	GLN	12	3.646	62.996	19.845	1.00	42.86
ATOM	34	CB	GLN	12	2.972	64.368	19.715	1.00	44.49
ATOM	35	CG	GLN	12	2.833	64.840	18.259	1.00	46.49
ATOM	36	CD	GLN	12	1.986	66.099	18.113	1.00	47.74
ATOM	37	OE1	GLN	12	2.055	66.799	17.088	1.00	48.30
ATOM	38	NE2	GLN	12	1.174	66.388	19.131	1.00	47.51
ATOM	39	C	GLN	12	5.014	63.023	19.192	1.00	41.14
ATOM	40	O	GLN	12	5.139	62.739	18.002	1.00	41.76
ATOM	41	N	ILE	13	6.038	63.360	19.971	1.00	38.51
ATOM	42	CA	ILE	13	7.398	63.388	19.450	1.00	36.48
ATOM	43	CB	ILE	13	8.274	64.351	20.261	1.00	35.85
ATOM	44	CG2	ILE	13	9.731	64.228	19.827	1.00	35.71
ATOM	45	CG1	ILE	13	7.740	65.777	20.079	1.00	35.77
ATOM	46	CD1	ILE	13	8.584	66.867	20.710	1.00	35.91
ATOM	47	C	ILE	13	8.018	61.981	19.452	1.00	36.01
ATOM	48	O	ILE	13	8.572	61.528	18.442	1.00	35.99
ATOM	49	N	LEU	14	7.903	61.288	20.580	1.00	34.88
ATOM	50	CA	LEU	14	8.430	59.934	20.711	1.00	33.91
ATOM	51	CB	LEU	14	8.230	59.432	22.141	1.00	33.29
ATOM	52	CG	LEU	14	8.853	60.321	23.215	1.00	33.43
ATOM	53	CD1	LEU	14	8.510	59.781	24.594	1.00	33.04

Figure 4   Sheet 2 of 62

ATOM	54	CD2	LEU	14	10.354	60.398	23.001	1.00	33.04
ATOM	55	C	LEU	14	7.766	58.957	19.730	1.00	33.55
ATOM	56	O	LEU	14	8.208	57.812	19.578	1.00	33.21
ATOM	57	N	ALA	15	6.710	59.403	19.065	1.00	32.69
ATOM	58	CA	ALA	15	6.021	58.551	18.104	1.00	32.59
ATOM	59	CB	ALA	15	4.628	59.104	17.821	1.00	31.95
ATOM	60	C	ALA	15	6.838	58.449	16.808	1.00	32.79
ATOM	61	O	ALA	15	6.664	57.519	16.018	1.00	33.05
ATOM	62	N	GLU	16	7.746	59.395	16.599	1.00	32.33
ATOM	63	CA	GLU	16	8.575	59.369	15.403	1.00	32.74
ATOM	64	CB	GLU	16	9.566	60.531	15.401	1.00	34.23
ATOM	65	CG	GLU	16	8.950	61.910	15.298	1.00	38.39
ATOM	66	CD	GLU	16	10.017	62.998	15.162	1.00	41.11
ATOM	67	OE1	GLU	16	10.445	63.269	14.012	1.00	40.68
ATOM	68	OE2	GLU	16	10.438	63.562	16.212	1.00	42.77
ATOM	69	C	GLU	16	9.369	58.073	15.279	1.00	31.93
ATOM	70	O	GLU	16	9.570	57.568	14.179	1.00	33.41
ATOM	71	N	PHE	17	9.841	57.539	16.401	1.00	30.37
ATOM	72	CA	PHE	17	10.640	56.321	16.369	1.00	27.71
ATOM	73	CB	PHE	17	11.346	56.129	17.711	1.00	26.32
ATOM	74	CG	PHE	17	12.309	57.230	18.045	1.00	24.22
ATOM	75	CD1	PHE	17	11.846	58.500	18.389	1.00	23.88
ATOM	76	CD2	PHE	17	13.680	57.010	17.981	1.00	22.24
ATOM	77	CE1	PHE	17	12.741	59.531	18.660	1.00	22.63
ATOM	78	CE2	PHE	17	14.574	58.027	18.250	1.00	21.23
ATOM	79	CZ	PHE	17	14.105	59.291	18.589	1.00	22.01
ATOM	80	C	PHE	17	9.836	55.077	16.012	1.00	27.77
ATOM	81	O	PHE	17	10.400	54.004	15.802	1.00	27.38
ATOM	82	N	GLN	18	8.517	55.213	15.957	1.00	28.12
ATOM	83	CA	GLN	18	7.684	54.080	15.593	1.00	29.17
ATOM	84	CB	GLN	18	6.216	54.484	15.599	1.00	30.98
ATOM	85	CG	GLN	18	5.446	54.017	16.806	1.00	32.94
ATOM	86	CD	GLN	18	4.152	54.785	16.974	1.00	34.65
ATOM	87	OE1	GLN	18	3.389	54.976	16.014	1.00	37.17
ATOM	88	NE2	GLN	18	3.892	55.228	18.190	1.00	33.67
ATOM	89	C	GLN	18	8.068	53.602	14.193	1.00	28.97
ATOM	90	O	GLN	18	8.471	54.399	13.346	1.00	28.83
ATOM	91	N	LEU	19	7.931	52.298	13.971	1.00	29.02
ATOM	92	CA	LEU	19	8.235	51.659	12.704	1.00	29.94
ATOM	93	CB	LEU	19	9.641	51.069	12.749	1.00	29.78
ATOM	94	CG	LEU	19	10.782	51.813	12.037	1.00	30.77
ATOM	95	CD1	LEU	19	10.886	53.251	12.477	1.00	30.67
ATOM	96	CD2	LEU	19	12.083	51.087	12.339	1.00	32.05
ATOM	97	C	LEU	19	7.199	50.549	12.511	1.00	31.41
ATOM	98	O	LEU	19	7.288	49.484	13.137	1.00	31.35
ATOM	99	N	GLN	20	6.205	50.801	11.663	1.00	32.64
ATOM	100	CA	GLN	20	5.153	49.817	11.422	1.00	34.95
ATOM	101	CB	GLN	20	4.024	50.413	10.570	1.00	35.78
ATOM	102	CG	GLN	20	3.301	51.622	11.175	1.00	37.65
ATOM	103	CD	GLN	20	3.048	51.486	12.669	1.00	39.03
ATOM	104	OE1	GLN	20	2.603	50.441	13.152	1.00	40.92
ATOM	105	NE2	GLN	20	3.324	52.552	13.410	1.00	40.04
ATOM	106	C	GLN	20	5.692	48.568	10.730	1.00	35.83
ATOM	107	O	GLN	20	6.827	48.547	10.247	1.00	36.56
ATOM	108	N	GLU	21	4.864	47.531	10.681	1.00	36.52
ATOM	109	CA	GLU	21	5.240	46.279	10.062	1.00	37.80
ATOM	110	CB	GLU	21	4.024	45.357	9.998	1.00	39.22

Figure 4 Sheet 3 of 62

ATOM	111	CG	GLU	21	4.298	43.898	9.625	1.00	42.88
ATOM	112	CD	GLU	21	4.568	43.009	10.844	1.00	44.63
ATOM	113	OE1	GLU	21	4.540	41.758	10.699	1.00	45.40
ATOM	114	OE2	GLU	21	4.810	43.564	11.943	1.00	45.89
ATOM	115	C	GLU	21	5.770	46.549	8.654	1.00	38.20
ATOM	116	O	GLU	21	6.892	46.183	8.324	1.00	38.71
ATOM	117	N	GLU	22	4.972	47.208	7.826	1.00	38.54
ATOM	118	CA	GLU	22	5.386	47.478	6.457	1.00	39.08
ATOM	119	CB	GLU	22	4.308	48.267	5.703	1.00	40.61
ATOM	120	CG	GLU	22	3.123	47.406	5.313	1.00	43.51
ATOM	121	CD	GLU	22	3.556	46.039	4.773	1.00	45.80
ATOM	122	OE1	GLU	22	4.243	45.999	3.719	1.00	46.20
ATOM	123	OE2	GLU	22	3.215	45.007	5.414	1.00	46.87
ATOM	124	C	GLU	22	6.711	48.197	6.359	1.00	38.74
ATOM	125	O	GLU	22	7.482	47.954	5.423	1.00	39.26
ATOM	126	N	ASP	23	6.988	49.084	7.308	1.00	37.74
ATOM	127	CA	ASP	23	8.258	49.795	7.276	1.00	37.23
ATOM	128	CB	ASP	23	8.356	50.779	8.437	1.00	38.62
ATOM	129	CG	ASP	23	7.240	51.789	8.427	1.00	40.46
ATOM	130	OD1	ASP	23	7.104	52.508	7.408	1.00	41.26
ATOM	131	OD2	ASP	23	6.495	51.861	9.438	1.00	41.77
ATOM	132	C	ASP	23	9.371	48.760	7.382	1.00	35.54
ATOM	133	O	ASP	23	10.267	48.698	6.536	1.00	35.43
ATOM	134	N	LEU	24	9.294	47.937	8.420	1.00	33.31
ATOM	135	CA	LEU	24	10.288	46.910	8.631	1.00	32.04
ATOM	136	CB	LEU	24	9.898	46.062	9.842	1.00	31.35
ATOM	137	CG	LEU	24	9.920	46.801	11.196	1.00	31.20
ATOM	138	CD1	LEU	24	9.710	45.815	12.343	1.00	29.48
ATOM	139	CD2	LEU	24	11.253	47.526	11.367	1.00	31.51
ATOM	140	C	LEU	24	10.509	46.041	7.385	1.00	31.61
ATOM	141	O	LEU	24	11.645	45.723	7.049	1.00	31.67
ATOM	142	N	LYS	25	9.434	45.673	6.693	1.00	31.58
ATOM	143	CA	LYS	25	9.551	44.863	5.486	1.00	31.41
ATOM	144	CB	LYS	25	8.186	44.347	5.061	1.00	31.91
ATOM	145	CG	LYS	25	7.574	43.372	6.033	1.00	34.39
ATOM	146	CD	LYS	25	6.224	42.901	5.531	1.00	36.61
ATOM	147	CE	LYS	25	5.414	42.232	6.640	1.00	38.71
ATOM	148	NZ	LYS	25	3.978	42.086	6.235	1.00	39.39
ATOM	149	C	LYS	25	10.166	45.679	4.352	1.00	31.50
ATOM	150	O	LYS	25	10.969	45.170	3.568	1.00	30.92
ATOM	151	N	LYS	26	9.784	46.947	4.261	1.00	31.82
ATOM	152	CA	LYS	26	10.332	47.819	3.229	1.00	32.63
ATOM	153	CB	LYS	26	9.695	49.203	3.315	1.00	33.38
ATOM	154	CG	LYS	26	10.053	50.129	2.177	1.00	35.11
ATOM	155	CD	LYS	26	9.424	51.502	2.400	1.00	37.48
ATOM	156	CE	LYS	26	9.364	52.312	1.104	1.00	39.72
ATOM	157	NZ	LYS	26	8.706	53.645	1.307	1.00	42.62
ATOM	158	C	LYS	26	11.845	47.919	3.441	1.00	32.91
ATOM	159	O	LYS	26	12.614	48.012	2.479	1.00	32.90
ATOM	160	N	VAL	27	12.265	47.901	4.705	1.00	33.16
ATOM	161	CA	VAL	27	13.687	47.956	5.046	1.00	33.43
ATOM	162	CB	VAL	27	13.903	48.281	6.555	1.00	32.58
ATOM	163	CG1	VAL	27	15.335	47.960	6.963	1.00	32.13
ATOM	164	CG2	VAL	27	13.622	49.755	6.818	1.00	31.04
ATOM	165	C	VAL	27	14.305	46.586	4.727	1.00	33.90
ATOM	166	O	VAL	27	15.323	46.482	4.036	1.00	33.83
ATOM	167	N	MSE	28	13.668	45.536	5.223	1.00	34.26

Figure 4   Sheet 4 of 62

```
ATOM    168  CA   MSE    28      14.140  44.193   4.983  1.00  34.84
ATOM    169  CB   MSE    28      13.072  43.198   5.393  1.00  35.83
ATOM    170  CG   MSE    28      13.456  41.784   5.144  1.00  38.88
ATOM    171  SE   MSE    28      12.108  40.670   5.608  1.00  45.40
ATOM    172  CE   MSE    28      11.054  40.713   4.095  1.00  42.96
ATOM    173  C    MSE    28      14.465  44.016   3.505  1.00  35.32
ATOM    174  O    MSE    28      15.571  43.621   3.144  1.00  35.22
ATOM    175  N    ARG    29      13.495  44.331   2.655  1.00  36.22
ATOM    176  CA   ARG    29      13.665  44.191   1.218  1.00  36.59
ATOM    177  CB   ARG    29      12.352  44.520   0.509  1.00  37.37
ATOM    178  CG   ARG    29      11.223  43.542   0.827  1.00  38.96
ATOM    179  CD   ARG    29       9.913  43.960   0.152  1.00  40.89
ATOM    180  NE   ARG    29       8.760  43.281   0.744  1.00  42.88
ATOM    181  CZ   ARG    29       7.621  43.889   1.081  1.00  43.80
ATOM    182  NH1  ARG    29       7.475  45.201   0.881  1.00  43.07
ATOM    183  NH2  ARG    29       6.631  43.188   1.636  1.00  44.12
ATOM    184  C    ARG    29      14.814  45.008   0.625  1.00  36.30
ATOM    185  O    ARG    29      15.615  44.469  -0.133  1.00  35.58
ATOM    186  N    ARG    30      14.906  46.296   0.948  1.00  36.85
ATOM    187  CA   ARG    30      16.008  47.091   0.410  1.00  38.41
ATOM    188  CB   ARG    30      15.944  48.543   0.894  1.00  39.31
ATOM    189  CG   ARG    30      14.676  49.285   0.513  1.00  41.96
ATOM    190  CD   ARG    30      14.742  50.763   0.933  1.00  44.07
ATOM    191  NE   ARG    30      13.415  51.384   0.995  1.00  45.48
ATOM    192  CZ   ARG    30      13.179  52.628   1.416  1.00  45.93
ATOM    193  NH1  ARG    30      14.175  53.403   1.810  1.00  45.92
ATOM    194  NH2  ARG    30      11.937  53.091   1.467  1.00  45.68
ATOM    195  C    ARG    30      17.338  46.461   0.843  1.00  39.05
ATOM    196  O    ARG    30      18.286  46.404   0.061  1.00  38.99
ATOM    197  N    MSE    31      17.408  45.999   2.092  1.00  39.11
ATOM    198  CA   MSE    31      18.615  45.348   2.596  1.00  38.96
ATOM    199  CB   MSE    31      18.374  44.784   4.002  1.00  40.43
ATOM    200  CG   MSE    31      19.512  43.922   4.599  1.00  42.62
ATOM    201  SE   MSE    31      21.083  44.819   5.027  1.00  48.46
ATOM    202  CE   MSE    31      20.438  45.988   6.389  1.00  45.46
ATOM    203  C    MSE    31      18.901  44.209   1.633  1.00  38.25
ATOM    204  O    MSE    31      19.973  44.132   1.038  1.00  38.18
ATOM    205  N    GLN    32      17.915  43.334   1.478  1.00  37.93
ATOM    206  CA   GLN    32      18.037  42.199   0.589  1.00  37.33
ATOM    207  CB   GLN    32      16.708  41.475   0.480  1.00  36.41
ATOM    208  CG   GLN    32      16.219  40.905   1.780  1.00  37.04
ATOM    209  CD   GLN    32      15.304  39.723   1.561  1.00  37.28
ATOM    210  OE1  GLN    32´     15.740  38.682   1.072  1.00  38.23
ATOM    211  NE2  GLN    32      14.027  39.874   1.912  1.00  37.39
ATOM    212  C    GLN    32      18.475  42.641  -0.791  1.00  37.81
ATOM    213  O    GLN    32      19.215  41.929  -1.466  1.00  37.79
ATOM    214  N    LYS    33      18.019  43.819  -1.205  1.00  38.80
ATOM    215  CA   LYS    33      18.362  44.345  -2.516  1.00  39.85
ATOM    216  CB   LYS    33      17.525  45.588  -2.830  1.00  40.63
ATOM    217  CG   LYS    33      17.591  45.992  -4.298  1.00  42.21
ATOM    218  CD   LYS    33      16.924  47.336  -4.561  1.00  43.78
ATOM    219  CE   LYS    33      17.160  47.803  -6.006  1.00  44.42
ATOM    220  NZ   LYS    33      16.639  49.187  -6.256  1.00  44.23
ATOM    221  C    LYS    33      19.843  44.695  -2.574  1.00  40.37
ATOM    222  O    LYS    33      20.519  44.411  -3.564  1.00  40.53
ATOM    223  N    GLU    34      20.331  45.312  -1.500  1.00  40.59
ATOM    224  CA   GLU    34      21.730  45.712  -1.378  1.00  40.95
```

Figure 4   Sheet 5 of 62

```
ATOM    225  CB   GLU    34       21.912  46.641  -0.179  1.00  41.24
ATOM    226  CG   GLU    34       21.229  47.956  -0.359  1.00  41.42
ATOM    227  CD   GLU    34       21.476  48.506  -1.741  1.00  42.21
ATOM    228  OE1  GLU    34       22.650  48.810  -2.063  1.00  42.30
ATOM    229  OE2  GLU    34       20.493  48.613  -2.507  1.00  43.29
ATOM    230  C    GLU    34       22.667  44.528  -1.221  1.00  40.87
ATOM    231  O    GLU    34       23.770  44.527  -1.767  1.00  41.06
ATOM    232  N    MSE    35       22.233  43.534  -0.456  1.00  41.15
ATOM    233  CA   MSE    35       23.038  42.350  -0.232  1.00  41.36
ATOM    234  CB   MSE    35       22.289  41.354   0.648  1.00  41.62
ATOM    235  CG   MSE    35       22.320  41.711   2.117  1.00  43.28
ATOM    236  SE   MSE    35       21.428  40.506   3.120  1.00  46.51
ATOM    237  CE   MSE    35       22.217  38.947   2.587  1.00  45.63
ATOM    238  C    MSE    35       23.376  41.701  -1.554  1.00  41.91
ATOM    239  O    MSE    35       24.532  41.367  -1.824  1.00  42.73
ATOM    240  N    ASP    36       22.367  41.533  -2.395  1.00  42.15
ATOM    241  CA   ASP    36       22.593  40.898  -3.675  1.00  41.96
ATOM    242  CB   ASP    36       21.264  40.633  -4.369  1.00  43.56
ATOM    243  CG   ASP    36       21.446  39.947  -5.699  1.00  45.91
ATOM    244  OD1  ASP    36       21.821  40.652  -6.675  1.00  46.71
ATOM    245  OD2  ASP    36       21.232  38.707  -5.754  1.00  46.76
ATOM    246  C    ASP    36       23.502  41.717  -4.578  1.00  41.03
ATOM    247  O    ASP    36       24.406  41.178  -5.217  1.00  40.61
ATOM    248  N    ARG    37       23.257  43.021  -4.620  1.00  40.36
ATOM    249  CA   ARG    37       24.034  43.937  -5.446  1.00  39.76
ATOM    250  CB   ARG    37       23.498  45.355  -5.283  1.00  39.56
ATOM    251  CG   ARG    37       22.252  45.621  -6.112  1.00  40.04
ATOM    252  CD   ARG    37       21.465  46.815  -5.590  1.00  41.19
ATOM    253  NE   ARG    37       22.278  48.002  -5.307  1.00  41.70
ATOM    254  CZ   ARG    37       22.938  48.711  -6.221  1.00  42.38
ATOM    255  NH1  ARG    37       22.899  48.362  -7.505  1.00  42.59
ATOM    256  NH2  ARG    37       23.615  49.792  -5.851  1.00  41.94
ATOM    257  C    ARG    37       25.524  43.908  -5.152  1.00  39.94
ATOM    258  O    ARG    37       26.335  43.732  -6.059  1.00  40.39
ATOM    259  N    GLY    38       25.893  44.076  -3.890  1.00  39.94
ATOM    260  CA   GLY    38       27.305  44.063  -3.557  1.00  39.60
ATOM    261  C    GLY    38       27.933  42.689  -3.699  1.00  39.23
ATOM    262  O    GLY    38       29.163  42.546  -3.695  1.00  39.59
ATOM    263  N    LEU    39       27.087  41.677  -3.834  1.00  38.16
ATOM    264  CA   LEU    39       27.545  40.307  -3.960  1.00  37.65
ATOM    265  CB   LEU    39       26.428  39.376  -3.495  1.00  35.76
ATOM    266  CG   LEU    39       26.821  38.029  -2.900  1.00  34.52
ATOM    267  CD1  LEU    39       27.899  38.248  -1.857  1.00  33.52
ATOM    268  CD2  LEU    39       25.606  37.348  -2.284  1.00  32.44
ATOM    269  C    LEU    39       27.931  39.989  -5.407  1.00  39.20
ATOM    270  O    LEU    39       28.594  38.980  -5.681  1.00  39.88
ATOM    271  N    ARG    40       27.537  40.866  -6.329  1.00  40.51
ATOM    272  CA   ARG    40       27.809  40.656  -7.751  1.00  41.77
ATOM    273  CB   ARG    40       26.494  40.686  -8.526  1.00  42.80
ATOM    274  CG   ARG    40       25.735  39.392  -8.377  1.00  44.75
ATOM    275  CD   ARG    40       24.257  39.551  -8.636  1.00  46.47
ATOM    276  NE   ARG    40       23.639  38.239  -8.797  1.00  48.71
ATOM    277  CZ   ARG    40       22.331  38.034  -8.890  1.00  50.01
ATOM    278  NH1  ARG    40       21.497  39.064  -8.831  1.00  51.43
ATOM    279  NH2  ARG    40       21.861  36.804  -9.060  1.00  50.46
ATOM    280  C    ARG    40       28.802  41.623  -8.374  1.00  42.16
ATOM    281  O    ARG    40       28.783  42.819  -8.097  1.00  42.42
```

Figure 4   Sheet 6 of 62

```
ATOM    282  N    LEU   41      29.650  41.087   -9.247  1.00 42.03
ATOM    283  CA   LEU   41      30.689  41.864   -9.902  1.00 42.00
ATOM    284  CB   LEU   41      31.307  41.044  -11.041  1.00 42.00
ATOM    285  CG   LEU   41      32.577  41.650  -11.660  1.00 41.78
ATOM    286  CD1  LEU   41      33.638  41.836  -10.583  1.00 40.20
ATOM    287  CD2  LEU   41      33.087  40.747  -12.773  1.00 41.95
ATOM    288  C    LEU   41      30.278  43.237  -10.428  1.00 42.57
ATOM    289  O    LEU   41      30.920  44.243  -10.110  1.00 42.64
ATOM    290  N    GLU   42      29.219  43.292  -11.227  1.00 43.03
ATOM    291  CA   GLU   42      28.788  44.562  -11.803  1.00 44.63
ATOM    292  CB   GLU   42      27.494  44.369  -12.607  1.00 43.97
ATOM    293  CG   GLU   42      26.436  43.533  -11.922  1.00 44.02
ATOM    294  CD   GLU   42      26.546  42.057  -12.248  1.00 43.71
ATOM    295  OE1  GLU   42      27.673  41.527  -12.245  1.00 45.13
ATOM    296  OE2  GLU   42      25.504  41.416  -12.496  1.00 43.50
ATOM    297  C    GLU   42      28.616  45.714  -10.805  1.00 46.21
ATOM    298  O    GLU   42      28.963  46.860  -11.103  1.00 46.22
ATOM    299  N    THR   43      28.105  45.413   -9.616  1.00 47.90
ATOM    300  CA   THR   43      27.873  46.443   -8.608  1.00 49.10
ATOM    301  CB   THR   43      26.370  46.533   -8.285  1.00 48.63
ATOM    302  OG1  THR   43      25.772  45.242   -8.465  1.00 47.66
ATOM    303  CG2  THR   43      25.679  47.531   -9.192  1.00 48.90
ATOM    304  C    THR   43      28.629  46.226   -7.302  1.00 50.94
ATOM    305  O    THR   43      28.481  47.008   -6.362  1.00 51.52
ATOM    306  N    HIS   44      29.456  45.185   -7.249  1.00 52.58
ATOM    307  CA   HIS   44      30.204  44.854   -6.037  1.00 53.89
ATOM    308  CB   HIS   44      31.210  43.727   -6.311  1.00 54.68
ATOM    309  CG   HIS   44      32.552  44.208   -6.775  1.00 55.77
ATOM    310  CD2  HIS   44      33.748  44.257   -6.139  1.00 55.82
ATOM    311  ND1  HIS   44      32.758  44.772   -8.017  1.00 56.36
ATOM    312  CE1  HIS   44      34.020  45.146   -8.125  1.00 56.30
ATOM    313  NE2  HIS   44      34.643  44.845   -6.999  1.00 56.06
ATOM    314  C    HIS   44      30.950  46.013   -5.398  1.00 54.87
ATOM    315  O    HIS   44      30.823  46.254   -4.199  1.00 55.06
ATOM    316  N    GLU   45      31.724  46.732   -6.203  1.00 56.25
ATOM    317  CA   GLU   45      32.540  47.826   -5.703  1.00 57.17
ATOM    318  CB   GLU   45      33.618  48.180   -6.721  1.00 59.35
ATOM    319  CG   GLU   45      33.146  49.127   -7.800  1.00 61.61
ATOM    320  CD   GLU   45      34.107  50.279   -7.985  1.00 63.07
ATOM    321  OE1  GLU   45      35.228  50.038   -8.487  1.00 63.72
ATOM    322  OE2  GLU   45      33.747  51.420   -7.613  1.00 64.00
ATOM    323  C    GLU   45      31.762  49.074   -5.356  1.00 56.66
ATOM    324  O    GLU   45      32.295  49.985   -4.732  1.00 56.54
ATOM    325  N    GLU   46      30.508  49.135   -5.772  1.00 56.24
ATOM    326  CA   GLU   46      29.708  50.306   -5.456  1.00 56.37
ATOM    327  CB   GLU   46      29.542  51.157   -6.704  1.00 57.92
ATOM    328  CG   GLU   46      30.881  51.645   -7.212  1.00 60.77
ATOM    329  CD   GLU   46      30.782  52.400   -8.515  1.00 62.28
ATOM    330  OE1  GLU   46      30.566  51.762   -9.571  1.00 62.25
ATOM    331  OE2  GLU   46      30.914  53.641   -8.474  1.00 63.95
ATOM    332  C    GLU   46      28.366  49.891   -4.873  1.00 55.40
ATOM    333  O    GLU   46      27.309  50.123   -5.457  1.00 55.75
ATOM    334  N    ALA   47      28.440  49.264   -3.704  1.00 53.89
ATOM    335  CA   ALA   47      27.273  48.783   -2.987  1.00 51.80
ATOM    336  CB   ALA   47      27.140  47.280   -3.159  1.00 52.36
ATOM    337  C    ALA   47      27.470  49.111   -1.524  1.00 49.98
ATOM    338  O    ALA   47      28.448  48.664   -0.923  1.00 50.36
```

Figure 4   Sheet 7 of 62

```
ATOM    339  N    SER    48      26.553  49.894  -0.960  1.00  47.18
ATOM    340  CA   SER    48      26.630  50.267   0.444  1.00  44.70
ATOM    341  CB   SER    48      25.299  50.860   0.897  1.00  46.13
ATOM    342  OG   SER    48      24.243  49.927   0.720  1.00  47.87
ATOM    343  C    SER    48      26.965  49.041   1.287  1.00  42.45
ATOM    344  O    SER    48      27.841  49.082   2.147  1.00  42.01
ATOM    345  N    VAL    49      26.261  47.946   1.037  1.00  40.48
ATOM    346  CA   VAL    49      26.516  46.713   1.762  1.00  38.96
ATOM    347  CB   VAL    49      25.231  45.849   1.875  1.00  38.62
ATOM    348  CG1  VAL    49      25.496  44.625   2.740  1.00  38.40
ATOM    349  CG2  VAL    49      24.102  46.672   2.472  1.00  37.16
ATOM    350  C    VAL    49      27.572  45.997   0.929  1.00  37.97
ATOM    351  O    VAL    49      27.266  45.474  -0.137  1.00  38.42
ATOM    352  N    LYS    50      28.810  45.982   1.422  1.00  36.51
ATOM    353  CA   LYS    50      29.937  45.385   0.703  1.00  34.95
ATOM    354  CB   LYS    50      31.250  45.843   1.334  1.00  35.51
ATOM    355  CG   LYS    50      31.574  47.322   1.091  1.00  36.68
ATOM    356  CD   LYS    50      30.676  48.249   1.913  1.00  39.05
ATOM    357  CE   LYS    50      30.865  48.018   3.419  1.00  39.54
ATOM    358  NZ   LYS    50      32.316  48.157   3.792  1.00  40.04
ATOM    359  C    LYS    50      30.012  43.879   0.482  1.00  33.72
ATOM    360  O    LYS    50      30.845  43.421  -0.293  1.00  33.30
ATOM    361  N    MSE    51      29.171  43.100   1.147  1.00  33.02
ATOM    362  CA   MSE    51      29.209  41.647   0.967  1.00  32.08
ATOM    363  CB   MSE    51      28.291  41.257  -0.190  1.00  34.01
ATOM    364  CG   MSE    51      26.867  41.744  -0.025  1.00  36.03
ATOM    365  SE   MSE    51      26.148  41.146   1.529  1.00  40.73
ATOM    366  CE   MSE    51      25.558  39.411   1.085  1.00  37.98
ATOM    367  C    MSE    51      30.637  41.180   0.666  1.00  30.17
ATOM    368  O    MSE    51      30.928  40.723  -0.437  1.00  30.22
ATOM    369  N    LEU    52      31.518  41.295   1.650  1.00  28.96
ATOM    370  CA   LEU    52      32.920  40.928   1.487  1.00  27.43
ATOM    371  CB   LEU    52      33.769  41.839   2.357  1.00  28.05
ATOM    372  CG   LEU    52      33.649  43.319   1.991  1.00  28.52
ATOM    373  CD1  LEU    52      34.222  44.171   3.116  1.00  28.77
ATOM    374  CD2  LEU    52      34.369  43.583   0.658  1.00  28.75
ATOM    375  C    LEU    52      33.273  39.482   1.803  1.00  26.61
ATOM    376  O    LEU    52      32.997  38.995   2.893  1.00  25.26
ATOM    377  N    PRO    53      33.911  38.774   0.844  1.00  27.04
ATOM    378  CD   PRO    53      34.270  39.142  -0.540  1.00  25.69
ATOM    379  CA   PRO    53      34.264  37.375   1.133  1.00  27.99
ATOM    380  CB   PRO    53      34.807  36.864  -0.204  1.00  26.92
ATOM    381  CG   PRO    53      34.184  37.825  -1.241  1.00  25.77
ATOM    382  C    PRO    53      35.314  37.361   2.239  1.00  28.40
ATOM    383  O    PRO    53      36.152  38.271   2.317  1.00  28.36
ATOM    384  N    THR    54      35.255  36.329   3.080  1.00  29.46
ATOM    385  CA   THR    54      36.149  36.142   4.226  1.00  30.53
ATOM    386  CB   THR    54      35.317  35.951   5.502  1.00  29.48
ATOM    387  OG1  THR    54      34.589  34.711   5.418  1.00  27.97
ATOM    388  CG2  THR    54      34.324  37.084   5.659  1.00  29.42
ATOM    389  C    THR    54      37.018  34.884   4.071  1.00  31.60
ATOM    390  O    THR    54      37.657  34.423   5.025  1.00  32.25
ATOM    391  N    TYR    55      37.017  34.311   2.877  1.00  32.63
ATOM    392  CA   TYR    55      37.763  33.089   2.615  1.00  34.41
ATOM    393  CB   TYR    55      39.249  33.421   2.405  1.00  33.07
ATOM    394  CG   TYR    55      39.458  34.175   1.101  1.00  32.58
ATOM    395  CD1  TYR    55      39.518  35.571   1.067  1.00  32.44
```

Figure 4   Sheet 8 of 62

```
ATOM    396  CE1 TYR    55      39.572  36.263  -0.157  1.00  32.48
ATOM    397  CD2 TYR    55      39.467  33.492  -0.117  1.00  31.97
ATOM    398  CE2 TYR    55      39.516  34.172  -1.335  1.00  31.83
ATOM    399  CZ  TYR    55      39.566  35.548  -1.351  1.00  32.18
ATOM    400  OH  TYR    55      39.575  36.200  -2.568  1.00  32.67
ATOM    401  C   TYR    55      37.559  31.956   3.637  1.00  36.06
ATOM    402  O   TYR    55      38.314  30.991   3.665  1.00  37.61
ATOM    403  N   VAL    56      36.518  32.059   4.459  1.00  38.03
ATOM    404  CA  VAL    56      36.199  31.006   5.429  1.00  39.87
ATOM    405  CB  VAL    56      35.483  31.586   6.663  1.00  38.75
ATOM    406  CG1 VAL    56      35.202  30.492   7.669  1.00  38.10
ATOM    407  CG2 VAL    56      36.336  32.660   7.285  1.00  38.76
ATOM    408  C   VAL    56      35.249  30.032   4.706  1.00  42.20
ATOM    409  O   VAL    56      34.098  30.376   4.418  1.00  42.02
ATOM    410  N   ARG    57      35.718  28.821   4.414  1.00  44.49
ATOM    411  CA  ARG    57      34.896  27.860   3.676  1.00  47.07
ATOM    412  CB  ARG    57      35.688  27.288   2.499  1.00  48.02
ATOM    413  CG  ARG    57      36.209  28.310   1.508  1.00  49.08
ATOM    414  CD  ARG    57      36.558  27.626   0.185  1.00  49.69
ATOM    415  NE  ARG    57      37.239  28.528  -0.737  1.00  49.50
ATOM    416  CZ  ARG    57      38.367  29.167  -0.447  1.00  48.83
ATOM    417  NH1 ARG    57      38.938  28.997   0.745  1.00  48.13
ATOM    418  NH2 ARG    57      38.915  29.978  -1.345  1.00  47.51
ATOM    419  C   ARG    57      34.311  26.695   4.449  1.00  48.57
ATOM    420  O   ARG    57      34.810  26.310   5.500  1.00  48.65
ATOM    421  N   SER    58      33.256  26.117   3.891  1.00  51.15
ATOM    422  CA  SER    58      32.589  24.973   4.501  1.00  54.78
ATOM    423  CB  SER    58      31.204  24.793   3.882  1.00  54.26
ATOM    424  OG  SER    58      31.258  24.980   2.475  1.00  54.39
ATOM    425  C   SER    58      33.419  23.708   4.295  1.00  57.39
ATOM    426  O   SER    58      33.097  22.645   4.823  1.00  57.47
ATOM    427  N   THR    59      34.484  23.840   3.510  1.00  60.71
ATOM    428  CA  THR    59      35.392  22.740   3.216  1.00  64.02
ATOM    429  CB  THR    59      35.886  22.823   1.758  1.00  63.73
ATOM    430  OG1 THR    59      36.637  24.029   1.570  1.00  63.22
ATOM    431  CG2 THR    59      34.704  22.843   0.801  1.00  63.87
ATOM    432  C   THR    59      36.571  22.880   4.176  1.00  67.10
ATOM    433  O   THR    59      37.554  23.562   3.884  1.00  67.44
ATOM    434  N   PRO    60      36.480  22.238   5.349  1.00  69.75
ATOM    435  CD  PRO    60      35.366  21.412   5.854  1.00  70.63
ATOM    436  CA  PRO    60      37.556  22.320   6.337  1.00  71.72
ATOM    437  CB  PRO    60      36.841  21.982   7.636  1.00  71.72
ATOM    438  CG  PRO    60      35.909  20.881   7.182  1.00  71.50
ATOM    439  C   PRO    60      38.709  21.370   6.056  1.00  73.48
ATOM    440  O   PRO    60      39.522  21.609   5.158  1.00  73.53
ATOM    441  N   GLU    61      38.754  20.287   6.830  1.00  75.48
ATOM    442  CA  GLU    61      39.808  19.283   6.731  1.00  76.98
ATOM    443  CB  GLU    61      39.969  18.788   5.289  1.00  78.43
ATOM    444  CG  GLU    61      40.806  17.516   5.161  1.00  80.68
ATOM    445  CD  GLU    61      42.177  17.744   4.530  1.00  81.88
ATOM    446  OE1 GLU    61      42.993  18.498   5.100  1.00  82.28
ATOM    447  OE2 GLU    61      42.442  17.156   3.458  1.00  82.68
ATOM    448  C   GLU    61      41.083  19.969   7.194  1.00  77.00
ATOM    449  O   GLU    61      41.942  20.327   6.389  1.00  77.10
ATOM    450  N   GLY    62      41.177  20.181   8.502  1.00  76.85
ATOM    451  CA  GLY    62      42.344  20.826   9.069  1.00  76.72
ATOM    452  C   GLY    62      42.415  20.539  10.555  1.00  76.65
```

Figure 4   Sheet 9 of 62

```
ATOM   453  O    GLY  62    42.507  19.380  10.969  1.00  76.79
ATOM   454  N    SER  63    42.361  21.594  11.362  1.00  76.25
ATOM   455  CA   SER  63    42.417  21.458  12.814  1.00  75.06
ATOM   456  CB   SER  63    41.401  20.413  13.300  1.00  75.92
ATOM   457  OG   SER  63    41.350  20.363  14.718  1.00  76.69
ATOM   458  C    SER  63    43.818  21.062  13.259  1.00  73.60
ATOM   459  O    SER  63    44.090  19.899  13.561  1.00  73.10
ATOM   460  N    GLU  64    44.705  22.045  13.280  1.00  71.83
ATOM   461  CA   GLU  64    46.071  21.819  13.703  1.00  70.12
ATOM   462  CB   GLU  64    46.996  22.824  13.011  1.00  71.42
ATOM   463  CG   GLU  64    48.464  22.726  13.417  1.00  73.74
ATOM   464  CD   GLU  64    49.014  21.309  13.342  1.00  74.84
ATOM   465  OE1  GLU  64    48.623  20.466  14.187  1.00  75.26
ATOM   466  OE2  GLU  64    49.837  21.041  12.434  1.00  75.45
ATOM   467  C    GLU  64    46.136  21.971  15.221  1.00  67.97
ATOM   468  O    GLU  64    46.775  22.886  15.734  1.00  68.33
ATOM   469  N    VAL  65    45.448  21.076  15.927  1.00  65.13
ATOM   470  CA   VAL  65    45.400  21.067  17.391  1.00  62.32
ATOM   471  CB   VAL  65    45.335  19.621  17.918  1.00  62.48
ATOM   472  CG1  VAL  65    45.487  19.607  19.430  1.00  62.45
ATOM   473  CG2  VAL  65    44.011  18.975  17.508  1.00  62.79
ATOM   474  C    VAL  65    46.587  21.752  18.055  1.00  60.42
ATOM   475  O    VAL  65    47.703  21.708  17.540  1.00  60.54
ATOM   476  N    GLY  66    46.354  22.386  19.200  1.00  58.26
ATOM   477  CA   GLY  66    47.454  23.043  19.888  1.00  55.67
ATOM   478  C    GLY  66    47.081  24.174  20.823  1.00  53.42
ATOM   479  O    GLY  66    46.153  24.052  21.615  1.00  54.08
ATOM   480  N    ASP  67    47.832  25.267  20.739  1.00  51.06
ATOM   481  CA   ASP  67    47.614  26.460  21.549  1.00  48.67
ATOM   482  CB   ASP  67    48.617  26.531  22.703  1.00  49.14
ATOM   483  CG   ASP  67    48.381  25.462  23.751  1.00  49.34
ATOM   484  OD1  ASP  67    48.201  24.287  23.365  1.00  49.37
ATOM   485  OD2  ASP  67    48.386  25.791  24.956  1.00  49.62
ATOM   486  C    ASP  67    47.832  27.634  20.612  1.00  47.26
ATOM   487  O    ASP  67    48.786  27.635  19.827  1.00  47.44
ATOM   488  N    PHE  68    46.955  28.632  20.678  1.00  45.41
ATOM   489  CA   PHE  68    47.075  29.778  19.785  1.00  43.60
ATOM   490  CB   PHE  68    46.031  29.682  18.667  1.00  41.17
ATOM   491  CG   PHE  68    46.032  28.361  17.946  1.00  39.29
ATOM   492  CD1  PHE  68    45.621  27.199  18.592  1.00  38.55
ATOM   493  CD2  PHE  68    46.468  28.272  16.623  1.00  38.76
ATOM   494  CE1  PHE  68    45.647  25.966  17.934  1.00  38.24
ATOM   495  CE2  PHE  68    46.498  27.050  15.959  1.00  37.31
ATOM   496  CZ   PHE  68    46.086  25.893  16.619  1.00  37.76
ATOM   497  C    PHE  68    46.918  31.096  20.514  1.00  43.33
ATOM   498  O    PHE  68    46.395  31.147  21.621  1.00  43.27
ATOM   499  N    LEU  69    47.386  32.166  19.889  1.00  43.51
ATOM   500  CA   LEU  69    47.274  33.475  20.497  1.00  44.73
ATOM   501  CB   LEU  69    48.625  34.197  20.518  1.00  45.26
ATOM   502  CG   LEU  69    48.781  34.949  21.848  1.00  46.33
ATOM   503  CD1  LEU  69    49.166  33.928  22.932  1.00  46.09
ATOM   504  CD2  LEU  69    49.811  36.072  21.748  1.00  45.48
ATOM   505  C    LEU  69    46.275  34.278  19.681  1.00  45.37
ATOM   506  O    LEU  69    46.448  34.451  18.470  1.00  45.62
ATOM   507  N    SER  70    45.228  34.758  20.351  1.00  45.75
ATOM   508  CA   SER  70    44.177  35.528  19.697  1.00  44.98
ATOM   509  CB   SER  70    42.794  34.984  20.074  1.00  44.61
```

Figure 4   Sheet 10 of 62

```
ATOM    510  OG   SER    70      42.697  33.589  19.844  1.00 44.25
ATOM    511  C    SER    70      44.250  36.978  20.109  1.00 44.92
ATOM    512  O    SER    70      44.451  37.289  21.277  1.00 44.67
ATOM    513  N    LEU    71      44.095  37.858  19.130  1.00 45.85
ATOM    514  CA   LEU    71      44.092  39.294  19.366  1.00 47.27
ATOM    515  CB   LEU    71      45.064  40.000  18.421  1.00 47.71
ATOM    516  CG   LEU    71      46.552  39.942  18.787  1.00 49.06
ATOM    517  CD1  LEU    71      47.008  38.497  19.039  1.00 49.69
ATOM    518  CD2  LEU    71      47.348  40.572  17.656  1.00 49.35
ATOM    519  C    LEU    71      42.668  39.752  19.082  1.00 47.94
ATOM    520  O    LEU    71      41.873  38.997  18.499  1.00 48.06
ATOM    521  N    ASP    72      42.333  40.976  19.479  1.00 48.20
ATOM    522  CA   ASP    72      40.985  41.451  19.244  1.00 48.67
ATOM    523  CB   ASP    72      40.043  40.807  20.262  1.00 48.71
ATOM    524  CG   ASP    72      38.668  41.420  20.243  1.00 49.13
ATOM    525  OD1  ASP    72      38.090  41.549  19.144  1.00 49.57
ATOM    526  OD2  ASP    72      38.168  41.777  21.331  1.00 50.11
ATOM    527  C    ASP    72      40.819  42.962  19.258  1.00 48.98
ATOM    528  O    ASP    72      40.247  43.530  20.187  1.00 48.82
ATOM    529  N    LEU    73      41.312  43.613  18.214  1.00 49.73
ATOM    530  CA   LEU    73      41.193  45.060  18.117  1.00 51.48
ATOM    531  CB   LEU    73      42.199  45.603  17.096  1.00 50.80
ATOM    532  CG   LEU    73      42.160  47.096  16.774  1.00 50.07
ATOM    533  CD1  LEU    73      42.358  47.902  18.045  1.00 50.10
ATOM    534  CD2  LEU    73      43.223  47.421  15.738  1.00 49.97
ATOM    535  C    LEU    73      39.764  45.392  17.687  1.00 52.93
ATOM    536  O    LEU    73      38.909  44.507  17.628  1.00 52.38
ATOM    537  N    GLY    74      39.504  46.665  17.401  1.00 54.88
ATOM    538  CA   GLY    74      38.177  47.068  16.983  1.00 56.88
ATOM    539  C    GLY    74      37.285  47.420  18.148  1.00 58.48
ATOM    540  O    GLY    74      36.476  48.348  18.071  1.00 58.31
ATOM    541  N    GLY    75      37.428  46.668  19.233  1.00 60.27
ATOM    542  CA   GLY    75      36.621  46.925  20.410  1.00 62.46
ATOM    543  C    GLY    75      37.020  48.230  21.074  1.00 63.75
ATOM    544  O    GLY    75      37.824  49.005  20.536  1.00 64.06
ATOM    545  N    THR    76      36.452  48.481  22.248  1.00 64.50
ATOM    546  CA   THR    76      36.759  49.697  22.991  1.00 65.42
ATOM    547  CB   THR    76      35.905  49.776  24.266  1.00 66.28
ATOM    548  OG1  THR    76      36.361  48.791  25.203  1.00 67.43
ATOM    549  CG2  THR    76      34.425  49.505  23.938  1.00 66.14
ATOM    550  C    THR    76      38.238  49.651  23.385  1.00 65.25
ATOM    551  O    THR    76      39.005  50.595  23.152  1.00 65.01
ATOM    552  N    ASN    77      38.622  48.528  23.980  1.00 64.74
ATOM    553  CA   ASN    77      39.987  48.309  24.412  1.00 64.17
ATOM    554  CB   ASN    77      40.015  47.966  25.903  1.00 65.44
ATOM    555  CG   ASN    77      39.346  49.027  26.765  1.00 66.47
ATOM    556  OD1  ASN    77      39.656  50.219  26.663  1.00 67.13
ATOM    557  ND2  ASN    77      38.431  48.596  27.629  1.00 66.65
ATOM    558  C    ASN    77      40.547  47.149  23.603  1.00 63.19
ATOM    559  O    ASN    77      39.795  46.303  23.120  1.00 62.58
ATOM    560  N    PHE    78      41.866  47.123  23.446  1.00 62.14
ATOM    561  CA   PHE    78      42.526  46.051  22.708  1.00 61.12
ATOM    562  CB   PHE    78      43.887  46.514  22.172  1.00 61.81
ATOM    563  CG   PHE    78      44.684  45.420  21.516  1.00 62.50
ATOM    564  CD1  PHE    78      44.347  44.956  20.245  1.00 62.81
ATOM    565  CD2  PHE    78      45.741  44.818  22.189  1.00 62.99
ATOM    566  CE1  PHE    78      45.051  43.899  19.655  1.00 62.72
```

Figure 4   Sheet 11 of 62

```
ATOM   567  CE2 PHE    78    46.450  43.763  21.607  1.00  63.38
ATOM   568  CZ  PHE    78    46.103  43.301  20.336  1.00  63.01
ATOM   569  C   PHE    78    42.732  44.893  23.668  1.00  60.09
ATOM   570  O   PHE    78    43.065  45.100  24.834  1.00  60.08
ATOM   571  N   ARG    79    42.528  43.675  23.184  1.00  58.63
ATOM   572  CA  ARG    79    42.706  42.504  24.025  1.00  57.40
ATOM   573  CB  ARG    79    41.367  41.819  24.280  1.00  57.06
ATOM   574  CG  ARG    79    41.481  40.637  25.222  1.00  57.49
ATOM   575  CD  ARG    79    40.221  39.819  25.219  1.00  57.47
ATOM   576  NE  ARG    79    39.062  40.646  25.504  1.00  57.16
ATOM   577  CZ  ARG    79    37.818  40.266  25.267  1.00  57.69
ATOM   578  NH1 ARG    79    37.586  39.071  24.738  1.00  57.38
ATOM   579  NH2 ARG    79    36.812  41.080  25.555  1.00  58.45
ATOM   580  C   ARG    79    43.663  41.522  23.368  1.00  56.71
ATOM   581  O   ARG    79    43.926  41.619  22.170  1.00  57.24
ATOM   582  N   VAL    80    44.180  40.590  24.167  1.00  55.50
ATOM   583  CA  VAL    80    45.114  39.557  23.724  1.00  54.27
ATOM   584  CB  VAL    80    46.576  39.947  23.996  1.00  54.31
ATOM   585  CG1 VAL    80    47.491  38.779  23.674  1.00  54.49
ATOM   586  CG2 VAL    80    46.960  41.158  23.166  1.00  54.39
ATOM   587  C   VAL    80    44.806  38.327  24.555  1.00  54.04
ATOM   588  O   VAL    80    44.517  38.447  25.738  1.00  53.31
ATOM   589  N   MSE    81    44.881  37.144  23.957  1.00  54.52
ATOM   590  CA  MSE    81    44.568  35.935  24.703  1.00  54.59
ATOM   591  CB  MSE    81    43.053  35.804  24.828  1.00  57.08
ATOM   592  CG  MSE    81    42.300  36.025  23.520  1.00  60.39
ATOM   593  SE  MSE    81    40.534  36.437  23.792  1.00  65.62
ATOM   594  CE  MSE    81    39.999  34.926  24.679  1.00  62.03
ATOM   595  C   MSE    81    45.142  34.645  24.146  1.00  53.56
ATOM   596  O   MSE    81    45.598  34.582  23.007  1.00  52.99
ATOM   597  N   LEU    82    45.096  33.611  24.978  1.00  52.63
ATOM   598  CA  LEU    82    45.602  32.292  24.638  1.00  51.86
ATOM   599  CB  LEU    82    46.660  31.863  25.665  1.00  52.75
ATOM   600  CG  LEU    82    47.261  30.455  25.542  1.00  53.22
ATOM   601  CD1 LEU    82    48.562  30.521  24.736  1.00  52.42
ATOM   602  CD2 LEU    82    47.523  29.882  26.937  1.00  53.00
ATOM   603  C   LEU    82    44.461  31.286  24.650  1.00  51.18
ATOM   604  O   LEU    82    43.718  31.186  25.632  1.00  51.20
ATOM   605  N   VAL    83    44.333  30.535  23.563  1.00  50.58
ATOM   606  CA  VAL    83    43.292  29.522  23.448  1.00  50.00
ATOM   607  CB  VAL    83    42.274  29.887  22.362  1.00  49.63
ATOM   608  CG1 VAL    83    41.213  28.794  22.262  1.00  49.26
ATOM   609  CG2 VAL    83    41.660  31.244  22.670  1.00  48.32
ATOM   610  C   VAL    83    43.914  28.187  23.080  1.00  50.53
ATOM   611  O   VAL    83    44.759  28.122  22.192  1.00  50.93
ATOM   612  N   LYS    84    43.496  27.127  23.763  1.00  51.05
ATOM   613  CA  LYS    84    44.017  25.788  23.504  1.00  51.89
ATOM   614  CB  LYS    84    44.338  25.061  24.826  1.00  51.79
ATOM   615  CG  LYS    84    44.716  23.581  24.659  1.00  51.85
ATOM   616  CD  LYS    84    44.951  22.870  26.009  1.00  51.58
ATOM   617  CE  LYS    84    46.429  22.848  26.422  1.00  50.92
ATOM   618  NZ  LYS    84    47.041  24.198  26.592  1.00  50.33
ATOM   619  C   LYS    84    42.997  24.983  22.708  1.00  52.68
ATOM   620  O   LYS    84    42.115  24.327  23.282  1.00  53.00
ATOM   621  N   VAL    85    43.124  25.038  21.383  1.00  52.91
ATOM   622  CA  VAL    85    42.224  24.319  20.488  1.00  52.70
ATOM   623  CB  VAL    85    42.399  24.805  19.048  1.00  51.79
```

Figure 4   Sheet 12 of 62

```
ATOM    624  CG1 VAL    85      41.302  24.232  18.176  1.00 52.19
ATOM    625  CG2 VAL    85      42.389  26.319  19.017  1.00 51.59
ATOM    626  C   VAL    85      42.525  22.823  20.548  1.00 53.51
ATOM    627  O   VAL    85      43.637  22.389  20.243  1.00 53.87
ATOM    628  N   GLY    86      41.534  22.037  20.952  1.00 54.38
ATOM    629  CA  GLY    86      41.726  20.603  21.053  1.00 55.35
ATOM    630  C   GLY    86      40.901  19.810  20.060  1.00 56.21
ATOM    631  O   GLY    86      40.136  20.370  19.278  1.00 55.63
ATOM    632  N   GLU    87      41.050  18.493  20.106  1.00 57.81
ATOM    633  CA  GLU    87      40.339  17.611  19.195  1.00 59.64
ATOM    634  CB  GLU    87      41.290  16.529  18.673  1.00 60.88
ATOM    635  CG  GLU    87      40.680  15.648  17.611  1.00 62.26
ATOM    636  CD  GLU    87      40.215  16.457  16.423  1.00 63.21
ATOM    637  OE1 GLU    87      41.072  16.931  15.644  1.00 63.20
ATOM    638  OE2 GLU    87      38.989  16.631  16.278  1.00 64.58
ATOM    639  C   GLU    87      39.133  16.959  19.859  1.00 60.12
ATOM    640  O   GLU    87      39.271  16.187  20.810  1.00 60.00
ATOM    641  N   GLY    88      37.948  17.273  19.347  1.00 60.93
ATOM    642  CA  GLY    88      36.735  16.707  19.902  1.00 61.61
ATOM    643  C   GLY    88      35.840  16.120  18.833  1.00 62.11
ATOM    644  O   GLY    88      36.038  16.346  17.638  1.00 61.67
ATOM    645  N   GLU    89      34.845  15.363  19.274  1.00 62.79
ATOM    646  CA  GLU    89      33.898  14.724  18.372  1.00 63.90
ATOM    647  CB  GLU    89      32.782  14.089  19.203  1.00 63.50
ATOM    648  CG  GLU    89      33.304  13.137  20.275  1.00 62.64
ATOM    649  CD  GLU    89      32.214  12.623  21.203  1.00 62.46
ATOM    650  OE1 GLU    89      32.510  11.728  22.019  1.00 62.39
ATOM    651  OE2 GLU    89      31.064  13.110  21.128  1.00 62.11
ATOM    652  C   GLU    89      33.312  15.688  17.325  1.00 65.16
ATOM    653  O   GLU    89      32.975  16.837  17.634  1.00 64.98
ATOM    654  N   GLU    90      33.204  15.205  16.087  1.00 66.03
ATOM    655  CA  GLU    90      32.667  15.977  14.958  1.00 66.67
ATOM    656  CB  GLU    90      31.135  15.974  14.978  1.00 67.21
ATOM    657  CG  GLU    90      30.495  14.620  14.717  1.00 66.83
ATOM    658  CD  GLU    90      28.986  14.662  14.869  1.00 67.49
ATOM    659  OE1 GLU    90      28.308  15.273  14.009  1.00 67.17
ATOM    660  OE2 GLU    90      28.480  14.090  15.858  1.00 66.84
ATOM    661  C   GLU    90      33.149  17.421  14.871  1.00 66.91
ATOM    662  O   GLU    90      32.623  18.212  14.080  1.00 66.74
ATOM    663  N   GLY    91      34.149  17.769  15.671  1.00 67.05
ATOM    664  CA  GLY    91      34.649  19.126  15.628  1.00 67.38
ATOM    665  C   GLY    91      36.036  19.339  16.201  1.00 67.42
ATOM    666  O   GLY    91      37.025  18.797  15.708  1.00 68.24
ATOM    667  N   GLN    92      36.094  20.154  17.246  1.00 66.86
ATOM    668  CA  GLN    92      37.335  20.492  17.929  1.00 65.93
ATOM    669  CB  GLN    92      38.395  20.968  16.924  1.00 66.17
ATOM    670  CG  GLN    92      38.007  22.215  16.159  1.00 66.24
ATOM    671  CD  GLN    92      38.564  22.236  14.750  1.00 66.57
ATOM    672  OE1 GLN    92      38.432  21.260  14.007  1.00 66.37
ATOM    673  NE2 GLN    92      39.177  23.356  14.367  1.00 66.54
ATOM    674  C   GLN    92      36.999  21.605  18.920  1.00 65.21
ATOM    675  O   GLN    92      36.625  22.721  18.530  1.00 65.44
ATOM    676  N   TRP    93      37.111  21.278  20.204  1.00 63.62
ATOM    677  CA  TRP    93      36.820  22.227  21.261  1.00 61.61
ATOM    678  CB  TRP    93      36.859  21.540  22.626  1.00 62.77
ATOM    679  CG  TRP    93      38.050  20.641  22.857  1.00 63.86
ATOM    680  CD2 TRP    93      39.213  20.943  23.637  1.00 64.17
```

Figure 4   Sheet 13 of 62

ATOM	681	CE2	TRP	93	40.026	19.787	23.645	1.00	64.21
ATOM	682	CE3	TRP	93	39.647	22.080	24.336	1.00	64.11
ATOM	683	CD1	TRP	93	38.206	19.349	22.424	1.00	63.84
ATOM	684	NE1	TRP	93	39.387	18.830	22.897	1.00	63.69
ATOM	685	CZ2	TRP	93	41.246	19.731	24.324	1.00	64.43
ATOM	686	CZ3	TRP	93	40.859	22.026	25.009	1.00	64.63
ATOM	687	CH2	TRP	93	41.645	20.857	24.999	1.00	64.71
ATOM	688	C	TRP	93	37.784	23.393	21.248	1.00	59.53
ATOM	689	O	TRP	93	38.733	23.420	20.474	1.00	59.18
ATOM	690	N	SER	94	37.521	24.366	22.106	1.00	57.94
ATOM	691	CA	SER	94	38.353	25.549	22.207	1.00	56.46
ATOM	692	CB	SER	94	37.880	26.615	21.219	1.00	56.58
ATOM	693	OG	SER	94	36.504	26.899	21.412	1.00	56.78
ATOM	694	C	SER	94	38.185	26.050	23.624	1.00	55.56
ATOM	695	O	SER	94	37.142	25.822	24.237	1.00	55.36
ATOM	696	N	VAL	95	39.208	26.722	24.146	1.00	54.53
ATOM	697	CA	VAL	95	39.152	27.248	25.504	1.00	53.17
ATOM	698	CB	VAL	95	39.511	26.183	26.549	1.00	52.17
ATOM	699	CG1	VAL	95	39.742	26.844	27.891	1.00	52.13
ATOM	700	CG2	VAL	95	38.396	25.172	26.666	1.00	51.73
ATOM	701	C	VAL	95	40.099	28.399	25.719	1.00	52.74
ATOM	702	O	VAL	95	41.268	28.315	25.357	1.00	53.14
ATOM	703	N	LYS	96	39.587	29.469	26.318	1.00	52.63
ATOM	704	CA	LYS	96	40.402	30.637	26.629	1.00	52.93
ATOM	705	CB	LYS	96	39.513	31.849	26.932	1.00	53.25
ATOM	706	CG	LYS	96	40.277	33.129	27.231	1.00	53.79
ATOM	707	CD	LYS	96	39.910	33.706	28.595	1.00	54.80
ATOM	708	CE	LYS	96	38.427	34.102	28.682	1.00	55.69
ATOM	709	NZ	LYS	96	38.027	35.162	27.696	1.00	55.59
ATOM	710	C	LYS	96	41.154	30.218	27.882	1.00	52.96
ATOM	711	O	LYS	96	40.546	29.733	28.834	1.00	52.93
ATOM	712	N	THR	97	42.470	30.384	27.886	1.00	53.38
ATOM	713	CA	THR	97	43.253	29.980	29.050	1.00	53.93
ATOM	714	CB	THR	97	44.238	28.850	28.684	1.00	53.99
ATOM	715	OG1	THR	97	43.512	27.736	28.151	1.00	52.99
ATOM	716	CG2	THR	97	44.998	28.394	29.918	1.00	55.29
ATOM	717	C	THR	97	44.036	31.132	29.670	1.00	53.82
ATOM	718	O	THR	97	44.330	31.123	30.866	1.00	53.34
ATOM	719	N	LYS	98	44.373	32.117	28.848	1.00	53.85
ATOM	720	CA	LYS	98	45.115	33.276	29.315	1.00	54.60
ATOM	721	CB	LYS	98	46.627	33.096	29.087	1.00	55.51
ATOM	722	CG	LYS	98	47.220	31.809	29.652	1.00	56.78
ATOM	723	CD	LYS	98	47.074	31.733	31.162	1.00	58.23
ATOM	724	CE	LYS	98	47.553	30.389	31.713	1.00	58.82
ATOM	725	NZ	LYS	98	47.404	30.320	33.201	1.00	58.98
ATOM	726	C	LYS	98	44.644	34.479	28.518	1.00	54.54
ATOM	727	O	LYS	98	44.323	34.360	27.329	1.00	54.79
ATOM	728	N	HIS	99	44.590	35.632	29.173	1.00	54.03
ATOM	729	CA	HIS	99	44.193	36.853	28.496	1.00	54.03
ATOM	730	CB	HIS	99	42.720	36.793	28.052	1.00	55.02
ATOM	731	CG	HIS	99	41.732	36.872	29.172	1.00	55.71
ATOM	732	CD2	HIS	99	40.682	37.704	29.373	1.00	55.66
ATOM	733	ND1	HIS	99	41.739	35.999	30.239	1.00	56.19
ATOM	734	CE1	HIS	99	40.736	36.288	31.049	1.00	56.30
ATOM	735	NE2	HIS	99	40.080	37.319	30.546	1.00	56.72
ATOM	736	C	HIS	99	44.445	38.082	29.351	1.00	53.46
ATOM	737	O	HIS	99	44.526	38.007	30.577	1.00	53.47

Figure 4   Sheet 14 of 62

```
ATOM    738  N    GLN   100     44.583  39.214  28.683  1.00  52.94
ATOM    739  CA   GLN   100     44.841  40.468  29.349  1.00  53.34
ATOM    740  CB   GLN   100     46.354  40.649  29.513  1.00  53.39
ATOM    741  CG   GLN   100     46.790  42.001  30.055  1.00  54.26
ATOM    742  CD   GLN   100     46.168  42.345  31.394  1.00  54.43
ATOM    743  OE1  GLN   100     46.349  41.629  32.384  1.00  55.27
ATOM    744  NE2  GLN   100     45.433  43.452  31.432  1.00  53.60
ATOM    745  C    GLN   100     44.243  41.567  28.481  1.00  53.43
ATOM    746  O    GLN   100     44.416  41.569  27.260  1.00  53.75
ATOM    747  N    THR   101     43.527  42.493  29.105  1.00  52.90
ATOM    748  CA   THR   101     42.905  43.576  28.367  1.00  53.12
ATOM    749  CB   THR   101     41.495  43.826  28.894  1.00  52.52
ATOM    750  OG1  THR   101     40.789  42.582  28.925  1.00  52.85
ATOM    751  CG2  THR   101     40.752  44.808  27.999  1.00  52.23
ATOM    752  C    THR   101     43.731  44.845  28.499  1.00  53.61
ATOM    753  O    THR   101     44.285  45.108  29.563  1.00  53.95
ATOM    754  N    TYR   102     43.809  45.628  27.422  1.00  54.10
ATOM    755  CA   TYR   102     44.585  46.869  27.422  1.00  55.36
ATOM    756  CB   TYR   102     45.878  46.708  26.608  1.00  54.89
ATOM    757  CG   TYR   102     46.788  45.569  27.015  1.00  54.25
ATOM    758  CD1  TYR   102     46.382  44.241  26.888  1.00  54.08
ATOM    759  CE1  TYR   102     47.227  43.197  27.226  1.00  53.44
ATOM    760  CD2  TYR   102     48.069  45.822  27.497  1.00  53.79
ATOM    761  CE2  TYR   102     48.922  44.785  27.840  1.00  53.76
ATOM    762  CZ   TYR   102     48.498  43.475  27.701  1.00  53.85
ATOM    763  OH   TYR   102     49.355  42.442  28.021  1.00  54.03
ATOM    764  C    TYR   102     43.813  48.041  26.822  1.00  56.65
ATOM    765  O    TYR   102     43.173  47.899  25.781  1.00  56.91
ATOM    766  N    SER   103     43.891  49.203  27.462  1.00  58.50
ATOM    767  CA   SER   103     43.217  50.385  26.938  1.00  60.94
ATOM    768  CB   SER   103     42.997  51.411  28.049  1.00  61.09
ATOM    769  OG   SER   103     44.231  51.829  28.602  1.00  62.50
ATOM    770  C    SER   103     44.090  50.985  25.833  1.00  62.31
ATOM    771  O    SER   103     45.293  50.729  25.771  1.00  62.27
ATOM    772  N    ALA   104     43.487  51.783  24.960  1.00  64.47
ATOM    773  CA   ALA   104     44.226  52.386  23.856  1.00  67.01
ATOM    774  CB   ALA   104     43.516  52.093  22.526  1.00  67.01
ATOM    775  C    ALA   104     44.410  53.888  24.025  1.00  68.66
ATOM    776  O    ALA   104     43.458  54.658  23.902  1.00  69.01
ATOM    777  N    PRO   105     45.648  54.327  24.305  1.00  70.09
ATOM    778  CD   PRO   105     46.878  53.522  24.397  1.00  70.06
ATOM    779  CA   PRO   105     45.946  55.751  24.485  1.00  71.25
ATOM    780  CB   PRO   105     47.443  55.748  24.783  1.00  70.79
ATOM    781  CG   PRO   105     47.929  54.535  24.046  1.00  70.54
ATOM    782  C    PRO   105     45.592  56.586  23.251  1.00  72.81
ATOM    783  O    PRO   105     45.837  56.170  22.117  1.00  73.09
ATOM    784  N    GLU   106     45.012  57.762  23.479  1.00  74.39
ATOM    785  CA   GLU   106     44.619  58.652  22.391  1.00  76.25
ATOM    786  CB   GLU   106     43.991  59.921  22.950  1.00  76.77
ATOM    787  CG   GLU   106     42.702  59.673  23.680  1.00  78.35
ATOM    788  CD   GLU   106     42.397  60.775  24.657  1.00  79.28
ATOM    789  OE1  GLU   106     42.239  61.934  24.214  1.00  79.74
ATOM    790  OE2  GLU   106     42.326  60.478  25.871  1.00  80.03
ATOM    791  C    GLU   106     45.784  59.028  21.494  1.00  77.33
ATOM    792  O    GLU   106     45.600  59.262  20.300  1.00  77.48
ATOM    793  N    ASP   107     46.980  59.104  22.068  1.00  78.72
ATOM    794  CA   ASP   107     48.161  59.440  21.284  1.00  80.10
```

```
ATOM   795  CB   ASP  107    49.431  59.316  22.134  1.00  80.44
ATOM   796  CG   ASP  107    49.965  57.889  22.185  1.00  81.03
ATOM   797  OD1  ASP  107    49.198  56.976  22.569  1.00  81.42
ATOM   798  OD2  ASP  107    51.151  57.682  21.839  1.00  80.86
ATOM   799  C    ASP  107    48.212  58.424  20.151  1.00  80.92
ATOM   800  O    ASP  107    48.724  58.703  19.065  1.00  81.29
ATOM   801  N    ALA  108    47.670  57.241  20.428  1.00  81.68
ATOM   802  CA   ALA  108    47.628  56.151  19.463  1.00  82.45
ATOM   803  CB   ALA  108    47.605  54.813  20.200  1.00  82.45
ATOM   804  C    ALA  108    46.406  56.275  18.553  1.00  82.91
ATOM   805  O    ALA  108    46.536  56.351  17.331  1.00  82.98
ATOM   806  N    MSE  109    45.221  56.303  19.157  1.00  83.41
ATOM   807  CA   MSE  109    43.974  56.414  18.407  1.00  83.78
ATOM   808  CB   MSE  109    42.787  56.519  19.368  1.00  85.45
ATOM   809  CG   MSE  109    41.581  55.678  18.972  1.00  87.01
ATOM   810  SE   MSE  109    41.933  53.898  19.096  1.00  90.12
ATOM   811  CE   MSE  109    42.665  53.581  17.453  1.00  88.95
ATOM   812  C    MSE  109    43.992  57.633  17.494  1.00  83.17
ATOM   813  O    MSE  109    43.235  57.710  16.527  1.00  83.19
ATOM   814  N    THR  110    44.854  58.590  17.820  1.00  82.51
ATOM   815  CA   THR  110    44.986  59.815  17.040  1.00  82.00
ATOM   816  CB   THR  110    45.289  61.022  17.949  1.00  82.44
ATOM   817  OG1  THR  110    44.302  61.103  18.986  1.00  83.00
ATOM   818  CG2  THR  110    45.283  62.313  17.142  1.00  82.69
ATOM   819  C    THR  110    46.150  59.640  16.082  1.00  81.25
ATOM   820  O    THR  110    46.127  60.123  14.949  1.00  80.95
ATOM   821  N    GLY  111    47.168  58.933  16.559  1.00  80.84
ATOM   822  CA   GLY  111    48.358  58.691  15.768  1.00  80.12
ATOM   823  C    GLY  111    48.121  57.986  14.450  1.00  79.53
ATOM   824  O    GLY  111    47.018  57.531  14.148  1.00  79.54
ATOM   825  N    THR  112    49.181  57.904  13.658  1.00  78.87
ATOM   826  CA   THR  112    49.129  57.254  12.360  1.00  78.09
ATOM   827  CB   THR  112    50.427  57.553  11.561  1.00  78.67
ATOM   828  OG1  THR  112    50.329  57.001  10.240  1.00  79.18
ATOM   829  CG2  THR  112    51.644  56.956  12.279  1.00  78.48
ATOM   830  C    THR  112    48.992  55.748  12.579  1.00  77.09
ATOM   831  O    THR  112    49.231  55.254  13.685  1.00  76.48
ATOM   832  N    ALA  113    48.601  55.027  11.529  1.00  76.26
ATOM   833  CA   ALA  113    48.443  53.573  11.603  1.00  75.60
ATOM   834  CB   ALA  113    48.184  53.001  10.208  1.00  76.00
ATOM   835  C    ALA  113    49.711  52.965  12.191  1.00  74.65
ATOM   836  O    ALA  113    49.665  52.006  12.968  1.00  74.58
ATOM   837  N    GLU  114    50.845  53.538  11.803  1.00  73.24
ATOM   838  CA   GLU  114    52.139  53.088  12.288  1.00  71.57
ATOM   839  CB   GLU  114    53.246  53.971  11.700  1.00  72.34
ATOM   840  CG   GLU  114    53.130  54.167  10.188  1.00  71.64
ATOM   841  CD   GLU  114    53.325  52.877   9.401  1.00  72.49
ATOM   842  OE1  GLU  114    53.192  51.781   9.994  1.00  72.24
ATOM   843  OE2  GLU  114    53.600  52.960   8.183  1.00  71.83
ATOM   844  C    GLU  114    52.085  53.233  13.801  1.00  70.37
ATOM   845  O    GLU  114    52.297  52.266  14.537  1.00  69.92
ATOM   846  N    MET  115    51.778  54.450  14.246  1.00  68.75
ATOM   847  CA   MET  115    51.657  54.760  15.669  1.00  66.97
ATOM   848  CB   MET  115    51.013  56.140  15.866  1.00  67.15
ATOM   849  CG   MET  115    51.999  57.277  16.040  1.00  66.94
ATOM   850  SD   MET  115    53.203  56.869  17.320  1.00  67.61
ATOM   851  CE   MET  115    52.137  56.732  18.788  1.00  66.65
```

Figure 4   Sheet 16 of 62

ATOM	852	C	MET	115	50.799	53.718	16.374	1.00	65.81
ATOM	853	O	MET	115	51.266	53.010	17.275	1.00	65.94
ATOM	854	N	LEU	116	49.542	53.635	15.940	1.00	63.70
ATOM	855	CA	LEU	116	48.561	52.711	16.504	1.00	61.63
ATOM	856	CB	LEU	116	47.287	52.720	15.650	1.00	60.89
ATOM	857	CG	LEU	116	45.948	52.226	16.205	1.00	59.42
ATOM	858	CD1	LEU	116	44.953	52.182	15.051	1.00	58.84
ATOM	859	CD2	LEU	116	46.081	50.858	16.847	1.00	58.86
ATOM	860	C	LEU	116	49.083	51.285	16.613	1.00	60.35
ATOM	861	O	LEU	116	48.977	50.665	17.667	1.00	60.48
ATOM	862	N	PHE	117	49.641	50.756	15.531	1.00	59.14
ATOM	863	CA	PHE	117	50.138	49.391	15.580	1.00	58.14
ATOM	864	CB	PHE	117	50.298	48.819	14.173	1.00	57.03
ATOM	865	CG	PHE	117	49.055	48.144	13.669	1.00	56.22
ATOM	866	CD1	PHE	117	48.005	48.889	13.143	1.00	55.49
ATOM	867	CD2	PHE	117	48.909	46.763	13.783	1.00	55.59
ATOM	868	CE1	PHE	117	46.830	48.270	12.741	1.00	55.25
ATOM	869	CE2	PHE	117	47.736	46.134	13.384	1.00	55.20
ATOM	870	CZ	PHE	117	46.695	46.887	12.862	1.00	55.23
ATOM	871	C	PHE	117	51.415	49.204	16.382	1.00	57.89
ATOM	872	O	PHE	117	51.799	48.073	16.690	1.00	57.80
ATOM	873	N	ALA	118	52.078	50.303	16.725	1.00	57.35
ATOM	874	CA	ALA	118	53.275	50.193	17.537	1.00	56.79
ATOM	875	CB	ALA	118	54.004	51.533	17.594	1.00	56.42
ATOM	876	C	ALA	118	52.747	49.792	18.922	1.00	56.46
ATOM	877	O	ALA	118	53.220	48.829	19.536	1.00	56.68
ATOM	878	N	ALA	119	51.733	50.515	19.391	1.00	55.57
ATOM	879	CA	ALA	119	51.142	50.226	20.693	1.00	55.05
ATOM	880	CB	ALA	119	49.931	51.135	20.952	1.00	53.91
ATOM	881	C	ALA	119	50.719	48.769	20.763	1.00	54.96
ATOM	882	O	ALA	119	51.090	48.052	21.698	1.00	54.94
ATOM	883	N	ILE	120	49.948	48.338	19.763	1.00	55.10
ATOM	884	CA	ILE	120	49.443	46.969	19.715	1.00	55.51
ATOM	885	CB	ILE	120	48.679	46.679	18.397	1.00	54.45
ATOM	886	CG2	ILE	120	47.922	45.363	18.525	1.00	53.30
ATOM	887	CG1	ILE	120	47.688	47.808	18.089	1.00	53.32
ATOM	888	CD1	ILE	120	46.871	47.581	16.820	1.00	51.70
ATOM	889	C	ILE	120	50.575	45.957	19.846	1.00	56.57
ATOM	890	O	ILE	120	50.477	45.006	20.632	1.00	56.52
ATOM	891	N	SER	121	51.645	46.169	19.076	1.00	57.78
ATOM	892	CA	SER	121	52.814	45.284	19.093	1.00	58.54
ATOM	893	CB	SER	121	53.844	45.730	18.045	1.00	58.96
ATOM	894	OG	SER	121	53.377	45.507	16.720	1.00	59.32
ATOM	895	C	SER	121	53.457	45.280	20.473	1.00	58.74
ATOM	896	O	SER	121	54.007	44.265	20.918	1.00	57.56
ATOM	897	N	GLU	122	53.379	46.422	21.151	1.00	59.50
ATOM	898	CA	GLU	122	53.947	46.529	22.484	1.00	60.44
ATOM	899	CB	GLU	122	54.003	47.986	22.941	1.00	60.60
ATOM	900	CG	GLU	122	55.104	48.241	23.952	1.00	60.45
ATOM	901	CD	GLU	122	54.706	49.252	25.003	1.00	61.76
ATOM	902	OE1	GLU	122	54.152	50.312	24.630	1.00	61.92
ATOM	903	OE2	GLU	122	54.950	48.986	26.202	1.00	62.20
ATOM	904	C	GLU	122	53.091	45.725	23.452	1.00	60.63
ATOM	905	O	GLU	122	53.565	44.761	24.048	1.00	60.82
ATOM	906	N	CYS	123	51.831	46.120	23.605	1.00	60.96
ATOM	907	CA	CYS	123	50.936	45.410	24.510	1.00	61.79
ATOM	908	CB	CYS	123	49.481	45.840	24.278	1.00	61.63

Figure 4   Sheet 17 of 62

ATOM	909	SG	CYS	123	49.191	47.636	24.439	1.00	62.83
ATOM	910	C	CYS	123	51.107	43.922	24.233	1.00	61.90
ATOM	911	O	CYS	123	51.028	43.095	25.147	1.00	61.89
ATOM	912	N	ILE	124	51.350	43.588	22.966	1.00	62.36
ATOM	913	CA	ILE	124	51.561	42.197	22.588	1.00	62.79
ATOM	914	CB	ILE	124	52.033	42.061	21.109	1.00	62.52
ATOM	915	CG2	ILE	124	52.618	40.676	20.877	1.00	61.07
ATOM	916	CG1	ILE	124	50.866	42.280	20.138	1.00	61.53
ATOM	917	CD1	ILE	124	50.016	41.038	19.888	1.00	61.77
ATOM	918	C	ILE	124	52.673	41.706	23.499	1.00	62.76
ATOM	919	O	ILE	124	52.475	40.807	24.320	1.00	62.23
ATOM	920	N	SER	125	53.839	42.327	23.347	1.00	63.43
ATOM	921	CA	SER	125	55.020	42.002	24.138	1.00	64.63
ATOM	922	CB	SER	125	56.062	43.117	23.986	1.00	65.05
ATOM	923	OG	SER	125	57.324	42.745	24.523	1.00	67.01
ATOM	924	C	SER	125	54.646	41.840	25.610	1.00	64.32
ATOM	925	O	SER	125	54.886	40.794	26.219	1.00	64.46
ATOM	926	N	ASP	126	54.047	42.884	26.169	1.00	64.43
ATOM	927	CA	ASP	126	53.626	42.894	27.562	1.00	64.86
ATOM	928	CB	ASP	126	52.660	44.060	27.788	1.00	64.95
ATOM	929	CG	ASP	126	52.390	44.323	29.253	1.00	65.38
ATOM	930	OD1	ASP	126	51.952	43.389	29.955	1.00	65.74
ATOM	931	OD2	ASP	126	52.613	45.467	29.706	1.00	65.92
ATOM	932	C	ASP	126	52.968	41.572	27.980	1.00	64.65
ATOM	933	O	ASP	126	53.424	40.918	28.924	1.00	64.28
ATOM	934	N	PHE	127	51.902	41.189	27.274	1.00	64.96
ATOM	935	CA	PHE	127	51.177	39.948	27.565	1.00	65.21
ATOM	936	CB	PHE	127	50.145	39.657	26.468	1.00	64.22
ATOM	937	CG	PHE	127	49.569	38.258	26.525	1.00	63.67
ATOM	938	CD1	PHE	127	48.774	37.857	27.594	1.00	63.64
ATOM	939	CD2	PHE	127	49.830	37.343	25.512	1.00	63.42
ATOM	940	CE1	PHE	127	48.247	36.564	27.652	1.00	63.40
ATOM	941	CE2	PHE	127	49.308	36.051	25.560	1.00	63.55
ATOM	942	CZ	PHE	127	48.516	35.661	26.632	1.00	63.49
ATOM	943	C	PHE	127	52.154	38.791	27.631	1.00	65.83
ATOM	944	O	PHE	127	52.195	38.030	28.600	1.00	65.71
ATOM	945	N	LEU	128	52.931	38.684	26.562	1.00	66.57
ATOM	946	CA	LEU	128	53.942	37.656	26.387	1.00	67.52
ATOM	947	CB	LEU	128	54.773	38.022	25.166	1.00	67.64
ATOM	948	CG	LEU	128	53.926	38.452	23.969	1.00	67.42
ATOM	949	CD1	LEU	128	54.819	39.108	22.941	1.00	67.90
ATOM	950	CD2	LEU	128	53.195	37.251	23.387	1.00	67.65
ATOM	951	C	LEU	128	54.850	37.502	27.609	1.00	68.09
ATOM	952	O	LEU	128	54.829	36.468	28.285	1.00	67.92
ATOM	953	N	ASP	129	55.654	38.530	27.878	1.00	68.62
ATOM	954	CA	ASP	129	56.565	38.514	29.018	1.00	69.22
ATOM	955	CB	ASP	129	57.135	39.907	29.287	1.00	68.93
ATOM	956	CG	ASP	129	58.115	40.342	28.239	1.00	68.90
ATOM	957	OD1	ASP	129	59.100	39.606	28.011	1.00	69.12
ATOM	958	OD2	ASP	129	57.900	41.423	27.650	1.00	69.22
ATOM	959	C	ASP	129	55.843	38.059	30.267	1.00	69.59
ATOM	960	O	ASP	129	56.063	36.956	30.761	1.00	69.41
ATOM	961	N	LYS	130	54.973	38.940	30.753	1.00	70.10
ATOM	962	CA	LYS	130	54.190	38.733	31.958	1.00	70.67
ATOM	963	CB	LYS	130	53.285	39.946	32.159	1.00	70.80
ATOM	964	CG	LYS	130	54.076	41.252	32.052	1.00	70.54
ATOM	965	CD	LYS	130	53.218	42.479	32.266	1.00	70.22

Figure 4   Sheet 18 of 62

ATOM	966	CE	LYS	130	54.021	43.746	32.011	1.00	70.07
ATOM	967	NZ	LYS	130	53.204	44.977	32.195	1.00	69.69
ATOM	968	C	LYS	130	53.394	37.441	31.982	1.00	71.17
ATOM	969	O	LYS	130	52.381	37.331	32.673	1.00	70.99
ATOM	970	N	HIS	131	53.883	36.468	31.221	1.00	72.01
ATOM	971	CA	HIS	131	53.301	35.139	31.125	1.00	73.44
ATOM	972	CB	HIS	131	52.313	35.065	29.965	1.00	73.00
ATOM	973	CG	HIS	131	50.881	35.076	30.397	1.00	72.93
ATOM	974	CD2	HIS	131	49.960	34.085	30.454	1.00	72.73
ATOM	975	ND1	HIS	131	50.256	36.210	30.869	1.00	72.87
ATOM	976	CE1	HIS	131	49.010	35.917	31.196	1.00	73.01
ATOM	977	NE2	HIS	131	48.806	34.634	30.954	1.00	73.04
ATOM	978	C	HIS	131	54.424	34.124	30.908	1.00	74.61
ATOM	979	O	HIS	131	54.419	33.049	31.514	1.00	74.70
ATOM	980	N	GLN	132	55.374	34.502	30.046	1.00	76.14
ATOM	981	CA	GLN	132	56.566	33.727	29.658	1.00	77.30
ATOM	982	CB	GLN	132	56.536	32.293	30.218	1.00	77.68
ATOM	983	CG	GLN	132	55.424	31.387	29.676	1.00	78.41
ATOM	984	CD	GLN	132	55.823	30.611	28.436	1.00	78.88
ATOM	985	OE1	GLN	132	56.016	31.179	27.356	1.00	78.50
ATOM	986	NE2	GLN	132	55.951	29.294	28.587	1.00	79.41
ATOM	987	C	GLN	132	56.673	33.682	28.134	1.00	77.86
ATOM	988	O	GLN	132	57.769	33.638	27.574	1.00	77.91
ATOM	989	N	MSE	133	55.520	33.703	27.472	1.00	78.39
ATOM	990	CA	MSE	133	55.450	33.662	26.017	1.00	78.88
ATOM	991	CB	MSE	133	53.989	33.684	25.551	1.00	80.96
ATOM	992	CG	MSE	133	53.278	32.347	25.586	1.00	83.34
ATOM	993	SE	MSE	133	51.991	32.273	26.846	1.00	87.09
ATOM	994	CE	MSE	133	52.168	30.521	27.421	1.00	84.33
ATOM	995	C	MSE	133	56.174	34.812	25.333	1.00	77.90
ATOM	996	O	MSE	133	55.552	35.548	24.567	1.00	78.34
ATOM	997	N	LYS	134	57.470	34.973	25.587	1.00	75.97
ATOM	998	CA	LYS	134	58.225	36.053	24.949	1.00	73.96
ATOM	999	CB	LYS	134	58.976	36.879	25.997	1.00	73.14
ATOM	1000	CG	LYS	134	59.676	38.125	25.454	1.00	72.28
ATOM	1001	CD	LYS	134	58.697	39.250	25.141	1.00	70.99
ATOM	1002	CE	LYS	134	59.415	40.586	24.935	1.00	70.06
ATOM	1003	NZ	LYS	134	60.234	40.640	23.687	1.00	69.46
ATOM	1004	C	LYS	134	59.211	35.443	23.964	1.00	72.94
ATOM	1005	O	LYS	134	59.727	36.123	23.077	1.00	72.63
ATOM	1006	N	HIS	135	59.457	34.148	24.132	1.00	72.28
ATOM	1007	CA	HIS	135	60.377	33.411	23.275	1.00	71.52
ATOM	1008	CB	HIS	135	61.359	32.584	24.119	1.00	71.15
ATOM	1009	CG	HIS	135	60.719	31.448	24.859	1.00	70.88
ATOM	1010	CD2	HIS	135	60.908	30.109	24.773	1.00	70.87
ATOM	1011	ND1	HIS	135	59.750	31.635	25.822	1.00	70.81
ATOM	1012	CE1	HIS	135	59.370	30.462	26.298	1.00	70.56
ATOM	1013	NE2	HIS	135	60.057	29.519	25.678	1.00	70.85
ATOM	1014	C	HIS	135	59.584	32.482	22.365	1.00	71.26
ATOM	1015	O	HIS	135	60.152	31.818	21.499	1.00	71.53
ATOM	1016	N	LYS	136	58.272	32.434	22.574	1.00	70.85
ATOM	1017	CA	LYS	136	57.393	31.590	21.766	1.00	70.33
ATOM	1018	CB	LYS	136	56.077	31.329	22.508	1.00	69.64
ATOM	1019	CG	LYS	136	56.225	30.694	23.886	1.00	68.45
ATOM	1020	CD	LYS	136	56.740	29.271	23.783	1.00	68.01
ATOM	1021	CE	LYS	136	56.698	28.560	25.128	1.00	67.56
ATOM	1022	NZ	LYS	136	55.303	28.356	25.623	1.00	66.87

Figure 4   Sheet 19 of 62

```
ATOM  1023  C    LYS  136      57.088  32.296  20.443  1.00  70.46
ATOM  1024  O    LYS  136      57.100  33.530  20.371  1.00  70.94
ATOM  1025  N    LYS  137      56.828  31.519  19.396  1.00  70.16
ATOM  1026  CA   LYS  137      56.505  32.096  18.096  1.00  69.80
ATOM  1027  CB   LYS  137      57.505  31.642  17.023  1.00  71.09
ATOM  1028  CG   LYS  137      57.602  30.132  16.801  1.00  71.73
ATOM  1029  CD   LYS  137      58.567  29.840  15.654  1.00  72.44
ATOM  1030  CE   LYS  137      58.915  28.363  15.545  1.00  72.39
ATOM  1031  NZ   LYS  137      59.919  28.136  14.463  1.00  72.59
ATOM  1032  C    LYS  137      55.097  31.685  17.702  1.00  68.73
ATOM  1033  O    LYS  137      54.799  31.476  16.524  1.00  69.92
ATOM  1034  N    LEU  138      54.243  31.579  18.716  1.00  66.57
ATOM  1035  CA   LEU  138      52.841  31.193  18.586  1.00  63.82
ATOM  1036  CB   LEU  138      52.057  31.788  19.748  1.00  63.11
ATOM  1037  CG   LEU  138      52.364  31.145  21.092  1.00  62.89
ATOM  1038  CD1  LEU  138      51.924  32.068  22.220  1.00  62.68
ATOM  1039  CD2  LEU  138      51.669  29.786  21.150  1.00  61.80
ATOM  1040  C    LEU  138      52.114  31.553  17.294  1.00  62.26
ATOM  1041  O    LEU  138      52.416  32.566  16.647  1.00  62.54
ATOM  1042  N    PRO  139      51.149  30.708  16.894  1.00  60.11
ATOM  1043  CD   PRO  139      50.841  29.394  17.489  1.00  59.82
ATOM  1044  CA   PRO  139      50.356  30.937  15.682  1.00  57.91
ATOM  1045  CB   PRO  139      49.761  29.564  15.398  1.00  58.05
ATOM  1046  CG   PRO  139      49.573  28.999  16.772  1.00  59.12
ATOM  1047  C    PRO  139      49.302  31.968  16.101  1.00  55.89
ATOM  1048  O    PRO  139      48.469  31.693  16.973  1.00  55.71
ATOM  1049  N    LEU  140      49.358  33.154  15.501  1.00  53.40
ATOM  1050  CA   LEU  140      48.440  34.237  15.850  1.00  50.78
ATOM  1051  CB   LEU  140      49.195  35.576  15.834  1.00  49.87
ATOM  1052  CG   LEU  140      48.452  36.893  16.091  1.00  49.01
ATOM  1053  CD1  LEU  140      49.414  37.933  16.646  1.00  48.17
ATOM  1054  CD2  LEU  140      47.825  37.389  14.801  1.00  48.88
ATOM  1055  C    LEU  140      47.169  34.359  15.018  1.00  49.13
ATOM  1056  O    LEU  140      47.211  34.368  13.785  1.00  49.12
ATOM  1057  N    GLY  141      46.040  34.441  15.722  1.00  46.93
ATOM  1058  CA   GLY  141      44.743  34.613  15.086  1.00  43.70
ATOM  1059  C    GLY  141      44.324  36.041  15.402  1.00  41.11
ATOM  1060  O    GLY  141      44.277  36.414  16.569  1.00  41.46
ATOM  1061  N    PHE  142      44.018  36.842  14.388  1.00  38.27
ATOM  1062  CA   PHE  142      43.659  38.232  14.629  1.00  36.42
ATOM  1063  CB   PHE  142      44.648  39.118  13.882  1.00  34.58
ATOM  1064  CG   PHE  142      44.403  40.593  14.037  1.00  33.28
ATOM  1065  CD1  PHE  142      43.941  41.124  15.229  1.00  32.86
ATOM  1066  CD2  PHE  142      44.702  41.465  12.992  1.00  32.75
ATOM  1067  CE1  PHE  142      43.784  42.505  15.375  1.00  32.95
ATOM  1068  CE2  PHE  142      44.551  42.845  13.125  1.00  31.57
ATOM  1069  CZ   PHE  142      44.094  43.365  14.313  1.00  32.24
ATOM  1070  C    PHE  142      42.224  38.652  14.300  1.00  36.83
ATOM  1071  O    PHE  142      41.843  38.801  13.124  1.00  36.76
ATOM  1072  N    THR  143      41.423  38.848  15.347  1.00  35.96
ATOM  1073  CA   THR  143      40.047  39.288  15.156  1.00  34.35
ATOM  1074  CB   THR  143      39.179  38.997  16.373  1.00  33.98
ATOM  1075  OG1  THR  143      38.947  37.586  16.472  1.00  33.45
ATOM  1076  CG2  THR  143      37.854  39.750  16.255  1.00  33.35
ATOM  1077  C    THR  143      40.081  40.793  14.964  1.00  33.92
ATOM  1078  O    THR  143      40.190  41.544  15.928  1.00  34.30
ATOM  1079  N    PHE  144      40.009  41.227  13.716  1.00  33.00
```

Figure 4   Sheet 20 of 62

```
ATOM   1080  CA   PHE   144    40.029  42.649  13.383  1.00 31.69
ATOM   1081  CB   PHE   144    40.891  42.842  12.132  1.00 29.18
ATOM   1082  CG   PHE   144    41.189  44.264  11.807  1.00 26.95
ATOM   1083  CD1  PHE   144    41.727  45.108  12.763  1.00 26.21
ATOM   1084  CD2  PHE   144    40.956  44.755  10.533  1.00 25.39
ATOM   1085  CE1  PHE   144    42.026  46.428  12.450  1.00 26.79
ATOM   1086  CE2  PHE   144    41.250  46.070  10.212  1.00 25.46
ATOM   1087  CZ   PHE   144    41.785  46.910  11.167  1.00 25.80
ATOM   1088  C    PHE   144    38.562  42.981  13.112  1.00 32.02
ATOM   1089  O    PHE   144    37.929  42.280  12.333  1.00 33.96
ATOM   1090  N    SER   145    38.025  44.027  13.744  1.00 32.29
ATOM   1091  CA   SER   145    36.602  44.387  13.600  1.00 31.56
ATOM   1092  CB   SER   145    35.993  44.689  14.968  1.00 31.79
ATOM   1093  OG   SER   145    35.997  43.539  15.790  1.00 33.15
ATOM   1094  C    SER   145    36.271  45.546  12.679  1.00 30.95
ATOM   1095  O    SER   145    35.601  46.508  13.082  1.00 30.63
ATOM   1096  N    PHE   146    36.723  45.456  11.439  1.00 30.27
ATOM   1097  CA   PHE   146    36.452  46.513  10.489  1.00 29.49
ATOM   1098  CB   PHE   146    37.573  47.541  10.535  1.00 29.01
ATOM   1099  CG   PHE   146    37.848  48.054  11.908  1.00 27.96
ATOM   1100  CD1  PHE   146    38.654  47.336  12.775  1.00 28.87
ATOM   1101  CD2  PHE   146    37.245  49.221  12.359  1.00 27.88
ATOM   1102  CE1  PHE   146    38.852  47.777  14.078  1.00 29.72
ATOM   1103  CE2  PHE   146    37.434  49.670  13.659  1.00 26.92
ATOM   1104  CZ   PHE   146    38.232  48.955  14.520  1.00 28.49
ATOM   1105  C    PHE   146    36.318  45.937   9.093  1.00 29.49
ATOM   1106  O    PHE   146    36.668  44.778   8.846  1.00 29.56
ATOM   1107  N    PRO   147    35.805  46.738   8.152  1.00 29.02
ATOM   1108  CD   PRO   147    35.452  48.167   8.211  1.00 28.09
ATOM   1109  CA   PRO   147    35.662  46.212   6.798  1.00 30.12
ATOM   1110  CB   PRO   147    34.852  47.309   6.099  1.00 28.65
ATOM   1111  CG   PRO   147    35.377  48.540   6.749  1.00 28.13
ATOM   1112  C    PRO   147    37.047  45.969   6.179  1.00 30.89
ATOM   1113  O    PRO   147    37.938  46.821   6.263  1.00 32.17
ATOM   1114  N    VAL   148    37.221  44.807   5.557  1.00 31.62
ATOM   1115  CA   VAL   148    38.499  44.453   4.957  1.00 32.00
ATOM   1116  CB   VAL   148    39.399  43.733   6.002  1.00 32.44
ATOM   1117  CG1  VAL   148    40.471  42.940   5.311  1.00 33.36
ATOM   1118  CG2  VAL   148    40.035  44.758   6.934  1.00 32.04
ATOM   1119  C    VAL   148    38.351  43.557   3.733  1.00 31.54
ATOM   1120  O    VAL   148    37.937  42.402   3.858  1.00 30.91
ATOM   1121  N    ALA   149    38.688  44.091   2.560  1.00 31.66
ATOM   1122  CA   ALA   149    38.610  43.316   1.324  1.00 32.33
ATOM   1123  CB   ALA   149    38.834  44.213   0.120  1.00 31.16
ATOM   1124  C    ALA   149    39.723  42.288   1.428  1.00 33.43
ATOM   1125  O    ALA   149    40.882  42.653   1.431  1.00 35.59
ATOM   1126  N    HIS   150    39.387  41.008   1.535  1.00 33.73
ATOM   1127  CA   HIS   150    40.410  39.980   1.666  1.00 33.88
ATOM   1128  CB   HIS   150    39.868  38.780   2.450  1.00 34.82
ATOM   1129  CG   HIS   150    39.879  38.961   3.933  1.00 35.58
ATOM   1130  CD2  HIS   150    40.344  38.162   4.921  1.00 36.49
ATOM   1131  ND1  HIS   150    39.329  40.061   4.555  1.00 36.45
ATOM   1132  CE1  HIS   150    39.454  39.930   5.865  1.00 36.79
ATOM   1133  NE2  HIS   150    40.067  38.786   6.114  1.00 36.38
ATOM   1134  C    HIS   150    40.960  39.442   0.353  1.00 34.39
ATOM   1135  O    HIS   150    40.245  39.364  -0.655  1.00 34.56
ATOM   1136  N    ALA   151    42.239  39.068   0.380  1.00 34.73
```

Figure 4   Sheet 21 of 62

```
ATOM   1137  CA   ALA   151      42.898  38.440  -0.762  1.00  34.53
ATOM   1138  CB   ALA   151      44.334  38.949  -0.919  1.00  34.86
ATOM   1139  C    ALA   151      42.894  36.968  -0.338  1.00  34.46
ATOM   1140  O    ALA   151      42.734  36.065  -1.161  1.00  34.16
ATOM   1141  N    ASP   152      43.050  36.754   0.970  1.00  34.36
ATOM   1142  CA   ASP   152      43.045  35.422   1.562  1.00  35.45
ATOM   1143  CB   ASP   152      44.335  34.687   1.214  1.00  37.69
ATOM   1144  CG   ASP   152      44.233  33.185   1.431  1.00  40.20
ATOM   1145  OD1  ASP   152      43.219  32.717   2.007  1.00  40.73
ATOM   1146  OD2  ASP   152      45.177  32.464   1.018  1.00  42.29
ATOM   1147  C    ASP   152      42.901  35.549   3.088  1.00  35.53
ATOM   1148  O    ASP   152      43.048  36.642   3.642  1.00  35.08
ATOM   1149  N    ILE   153      42.627  34.433   3.762  1.00  35.49
ATOM   1150  CA   ILE   153      42.436  34.427   5.213  1.00  35.75
ATOM   1151  CB   ILE   153      42.258  32.984   5.754  1.00  35.32
ATOM   1152  CG2  ILE   153      43.609  32.316   5.937  1.00  34.16
ATOM   1153  CG1  ILE   153      41.593  33.022   7.130  1.00  35.44
ATOM   1154  CD1  ILE   153      40.225  33.697   7.131  1.00  36.43
ATOM   1155  C    ILE   153      43.571  35.079   6.011  1.00  36.77
ATOM   1156  O    ILE   153      43.450  35.278   7.229  1.00  36.40
ATOM   1157  N    ASP   154      44.665  35.411   5.332  1.00  37.10
ATOM   1158  CA   ASP   154      45.815  36.003   6.000  1.00  37.27
ATOM   1159  CB   ASP   154      46.982  35.013   5.991  1.00  38.98
ATOM   1160  CG   ASP   154      47.795  35.079   4.703  1.00  41.58
ATOM   1161  OD1  ASP   154      47.215  34.890   3.605  1.00  42.46
ATOM   1162  OD2  ASP   154      49.022  35.331   4.789  1.00  42.65
ATOM   1163  C    ASP   154      46.233  37.287   5.307  1.00  36.74
ATOM   1164  O    ASP   154      47.360  37.751   5.471  1.00  37.07
ATOM   1165  N    ALA   155      45.328  37.865   4.531  1.00  35.91
ATOM   1166  CA   ALA   155      45.650  39.093   3.830  1.00  36.20
ATOM   1167  CB   ALA   155      46.522  38.771   2.621  1.00  36.22
ATOM   1168  C    ALA   155      44.412  39.864   3.387  1.00  36.20
ATOM   1169  O    ALA   155      43.490  39.289   2.820  1.00  36.87
ATOM   1170  N    GLY   156      44.402  41.168   3.642  1.00  36.26
ATOM   1171  CA   GLY   156      43.279  41.997   3.245  1.00  37.08
ATOM   1172  C    GLY   156      43.481  43.446   3.647  1.00  38.10
ATOM   1173  O    GLY   156      44.027  43.727   4.711  1.00  38.52
ATOM   1174  N    ILE   157      43.052  44.377   2.805  1.00  39.16
ATOM   1175  CA   ILE   157      43.203  45.789   3.125  1.00  41.42
ATOM   1176  CB   ILE   157      43.389  46.646   1.842  1.00  42.84
ATOM   1177  CG2  ILE   157      44.844  46.550   1.349  1.00  44.32
ATOM   1178  CG1  ILE   157      42.399  46.193   0.761  1.00  43.93
ATOM   1179  CD1  ILE   157      42.630  46.838  -0.615  1.00  44.55
ATOM   1180  C    ILE   157      42.010  46.331   3.921  1.00  42.26
ATOM   1181  O    ILE   157      40.864  45.912   3.732  1.00  42.28
ATOM   1182  N    LEU   158      42.300  47.259   4.824  1.00  42.54
ATOM   1183  CA   LEU   158      41.283  47.873   5.648  1.00  43.22
ATOM   1184  CB   LEU   158      41.928  48.504   6.884  1.00  44.12
ATOM   1185  CG   LEU   158      41.090  49.514   7.670  1.00  44.84
ATOM   1186  CD1  LEU   158      40.020  48.782   8.472  1.00  45.23
ATOM   1187  CD2  LEU   158      42.006  50.320   8.590  1.00  45.09
ATOM   1188  C    LEU   158      40.548  48.947   4.855  1.00  43.56
ATOM   1189  O    LEU   158      40.984  50.099   4.801  1.00  43.77
ATOM   1190  N    LEU   159      39.434  48.569   4.239  1.00  43.40
ATOM   1191  CA   LEU   159      38.634  49.508   3.465  1.00  43.01
ATOM   1192  CB   LEU   159      37.238  48.935   3.280  1.00  43.36
ATOM   1193  CG   LEU   159      37.279  47.599   2.539  1.00  43.44
```

Figure 4   Sheet 22 of 62

```
ATOM   1194  CD1 LEU    159      36.020  46.808   2.829  1.00 44.00
ATOM   1195  CD2 LEU    159      37.443  47.857   1.050  1.00 42.93
ATOM   1196  C   LEU    159      38.564  50.879   4.139  1.00 42.62
ATOM   1197  O   LEU    159      38.745  51.905   3.488  1.00 43.03
ATOM   1198  N   ASN    160      38.297  50.902   5.440  1.00 42.20
ATOM   1199  CA  ASN    160      38.243  52.169   6.170  1.00 41.99
ATOM   1200  CB  ASN    160      37.347  53.197   5.447  1.00 42.23
ATOM   1201  CG  ASN    160      35.913  52.733   5.295  1.00 43.38
ATOM   1202  OD1 ASN    160      35.225  53.102   4.334  1.00 42.38
ATOM   1203  ND2 ASN    160      35.444  51.934   6.250  1.00 44.48
ATOM   1204  C   ASN    160      37.813  51.988   7.616  1.00 41.13
ATOM   1205  O   ASN    160      37.359  50.913   8.011  1.00 41.17
ATOM   1206  N   TRP    161      37.980  53.043   8.403  1.00 40.24
ATOM   1207  CA  TRP    161      37.652  53.004   9.824  1.00 39.69
ATOM   1208  CB  TRP    161      38.522  54.003  10.602  1.00 39.33
ATOM   1209  CG  TRP    161      39.987  53.640  10.769  1.00 39.07
ATOM   1210  CD2 TRP    161      40.527  52.469  11.411  1.00 38.63
ATOM   1211  CE2 TRP    161      41.931  52.616  11.438  1.00 38.27
ATOM   1212  CE3 TRP    161      39.960  51.317  11.972  1.00 38.43
ATOM   1213  CD1 TRP    161      41.060  54.417  10.436  1.00 38.40
ATOM   1214  NE1 TRP    161      42.228  53.812  10.840  1.00 38.42
ATOM   1215  CZ2 TRP    161      42.778  51.659  12.000  1.00 38.26
ATOM   1216  CZ3 TRP    161      40.809  50.357  12.538  1.00 38.07
ATOM   1217  CH2 TRP    161      42.200  50.540  12.545  1.00 38.37
ATOM   1218  C   TRP    161      36.196  53.301  10.150  1.00 39.07
ATOM   1219  O   TRP    161      35.578  54.193   9.562  1.00 39.38
ATOM   1220  N   THR    162      35.668  52.555  11.114  1.00 38.45
ATOM   1221  CA  THR    162      34.302  52.734  11.593  1.00 38.37
ATOM   1222  CB  THR    162      33.381  51.600  11.125  1.00 37.71
ATOM   1223  OG1 THR    162      33.926  50.338  11.548  1.00 37.02
ATOM   1224  CG2 THR    162      33.226  51.635   9.617  1.00 36.52
ATOM   1225  C   THR    162      34.357  52.702  13.121  1.00 38.24
ATOM   1226  O   THR    162      35.405  52.443  13.703  1.00 37.86
ATOM   1227  N   LYS    163      33.231  52.968  13.770  1.00 38.99
ATOM   1228  CA  LYS    163      33.192  52.941  15.222  1.00 39.72
ATOM   1229  CB  LYS    163      33.510  51.528  15.728  1.00 38.16
ATOM   1230  CG  LYS    163      32.467  50.487  15.311  1.00 36.62
ATOM   1231  CD  LYS    163      32.727  49.108  15.918  1.00 34.66
ATOM   1232  CE  LYS    163      33.829  48.349  15.195  1.00 33.22
ATOM   1233  NZ  LYS    163      34.068  47.031  15.850  1.00 32.19
ATOM   1234  C   LYS    163      34.142  53.956  15.848  1.00 40.71
ATOM   1235  O   LYS    163      34.690  53.723  16.931  1.00 40.69
ATOM   1236  N   GLY    164      34.338  55.076  15.156  1.00 41.81
ATOM   1237  CA  GLY    164      35.187  56.139  15.672  1.00 43.90
ATOM   1238  C   GLY    164      36.685  56.031  15.463  1.00 45.41
ATOM   1239  O   GLY    164      37.375  57.055  15.381  1.00 45.25
ATOM   1240  N   PHE    165      37.190  54.802  15.397  1.00 47.06
ATOM   1241  CA  PHE    165      38.613  54.560  15.197  1.00 48.70
ATOM   1242  CB  PHE    165      38.852  53.117  14.767  1.00 47.20
ATOM   1243  CG  PHE    165      39.290  52.222  15.870  1.00 45.64
ATOM   1244  CD1 PHE    165      38.443  51.937  16.929  1.00 45.87
ATOM   1245  CD2 PHE    165      40.544  51.632  15.833  1.00 45.19
ATOM   1246  CE1 PHE    165      38.840  51.064  17.945  1.00 46.28
ATOM   1247  CE2 PHE    165      40.952  50.763  16.834  1.00 45.80
ATOM   1248  CZ  PHE    165      40.098  50.475  17.896  1.00 45.96
ATOM   1249  C   PHE    165      39.250  55.471  14.154  1.00 50.94
ATOM   1250  O   PHE    165      38.633  55.823  13.143  1.00 50.36
```

Figure 4   Sheet 23 of 62

```
ATOM   1251  N    LYS  166    40.500  55.838  14.415  1.00  53.77
ATOM   1252  CA   LYS  166    41.275  56.680  13.514  1.00  56.56
ATOM   1253  CB   LYS  166    41.050  58.170  13.822  1.00  56.16
ATOM   1254  CG   LYS  166    39.720  58.697  13.290  1.00  56.44
ATOM   1255  CD   LYS  166    39.524  58.320  11.812  1.00  56.54
ATOM   1256  CE   LYS  166    38.131  58.694  11.305  1.00  56.74
ATOM   1257  NZ   LYS  166    37.863  58.198   9.922  1.00  56.86
ATOM   1258  C    LYS  166    42.751  56.322  13.640  1.00  58.33
ATOM   1259  O    LYS  166    43.180  55.747  14.651  1.00  58.69
ATOM   1260  N    ALA  167    43.510  56.647  12.597  1.00  59.76
ATOM   1261  CA   ALA  167    44.943  56.375  12.543  1.00  61.43
ATOM   1262  CB   ALA  167    45.220  54.901  12.834  1.00  60.92
ATOM   1263  C    ALA  167    45.401  56.725  11.137  1.00  62.76
ATOM   1264  O    ALA  167    45.147  55.967  10.197  1.00  63.38
ATOM   1265  N    SER  168    46.066  57.872  10.999  1.00  63.98
ATOM   1266  CA   SER  168    46.556  58.345   9.704  1.00  64.43
ATOM   1267  CB   SER  168    47.636  59.414   9.903  1.00  64.96
ATOM   1268  OG   SER  168    47.130  60.546  10.594  1.00  65.76
ATOM   1269  C    SER  168    47.115  57.216   8.846  1.00  64.59
ATOM   1270  O    SER  168    47.805  56.322   9.347  1.00  64.35
ATOM   1271  N    GLY  169    46.800  57.260   7.553  1.00  64.75
ATOM   1272  CA   GLY  169    47.280  56.245   6.632  1.00  65.55
ATOM   1273  C    GLY  169    47.158  54.821   7.142  1.00  65.88
ATOM   1274  O    GLY  169    48.151  54.097   7.255  1.00  65.72
ATOM   1275  N    ALA  170    45.936  54.416   7.465  1.00  66.32
ATOM   1276  CA   ALA  170    45.699  53.065   7.947  1.00  66.82
ATOM   1277  CB   ALA  170    44.930  53.100   9.256  1.00  66.65
ATOM   1278  C    ALA  170    44.890  52.346   6.879  1.00  67.02
ATOM   1279  O    ALA  170    45.209  51.226   6.477  1.00  67.31
ATOM   1280  N    GLU  171    43.847  53.017   6.410  1.00  66.85
ATOM   1281  CA   GLU  171    42.979  52.463   5.387  1.00  66.80
ATOM   1282  CB   GLU  171    41.705  53.292   5.287  1.00  67.90
ATOM   1283  CG   GLU  171    41.958  54.783   5.279  1.00  69.27
ATOM   1284  CD   GLU  171    40.850  55.552   4.590  1.00  70.17
ATOM   1285  OE1  GLU  171    40.789  55.506   3.340  1.00  70.45
ATOM   1286  OE2  GLU  171    40.038  56.191   5.296  1.00  70.67
ATOM   1287  C    GLU  171    43.666  52.427   4.032  1.00  65.92
ATOM   1288  O    GLU  171    44.469  53.301   3.711  1.00  66.22
ATOM   1289  N    GLY  172    43.339  51.408   3.242  1.00  64.69
ATOM   1290  CA   GLY  172    43.922  51.265   1.925  1.00  62.79
ATOM   1291  C    GLY  172    45.096  50.312   1.882  1.00  61.61
ATOM   1292  O    GLY  172    45.493  49.884   0.805  1.00  61.59
ATOM   1293  N    ASN  173    45.643  49.965   3.045  1.00  60.93
ATOM   1294  CA   ASN  173    46.800  49.065   3.115  1.00  60.42
ATOM   1295  CB   ASN  173    47.922  49.722   3.913  1.00  61.72
ATOM   1296  CG   ASN  173    48.035  51.201   3.631  1.00  62.78
ATOM   1297  OD1  ASN  173    48.367  51.605   2.515  1.00  63.29
ATOM   1298  ND2  ASN  173    47.741  52.024   4.637  1.00  63.06
ATOM   1299  C    ASN  173    46.463  47.747   3.771  1.00  59.26
ATOM   1300  O    ASN  173    45.440  47.624   4.430  1.00  59.57
ATOM   1301  N    ASN  174    47.336  46.763   3.598  1.00  58.79
ATOM   1302  CA   ASN  174    47.126  45.447   4.196  1.00  58.46
ATOM   1303  CB   ASN  174    48.264  44.495   3.793  1.00  57.45
ATOM   1304  CG   ASN  174    48.104  43.093   4.375  1.00  57.22
ATOM   1305  OD1  ASN  174    48.757  42.144   3.924  1.00  56.21
ATOM   1306  ND2  ASN  174    47.245  42.957   5.382  1.00  56.76
ATOM   1307  C    ASN  174    47.083  45.615   5.712  1.00  58.42
```

Figure 4   Sheet 24 of 62

```
ATOM   1308  O    ASN   174    47.927  46.302   6.281  1.00  59.03
ATOM   1309  N    VAL   175    46.091  45.008   6.359  1.00  58.23
ATOM   1310  CA   VAL   175    45.966  45.106   7.809  1.00  57.79
ATOM   1311  CB   VAL   175    44.544  44.765   8.295  1.00  57.69
ATOM   1312  CG1  VAL   175    44.461  44.933   9.807  1.00  56.81
ATOM   1313  CG2  VAL   175    43.531  45.665   7.603  1.00  57.69
ATOM   1314  C    VAL   175    46.944  44.150   8.470  1.00  57.62
ATOM   1315  O    VAL   175    47.734  44.560   9.319  1.00  57.89
ATOM   1316  N    VAL   176    46.896  42.878   8.086  1.00  57.24
ATOM   1317  CA   VAL   176    47.818  41.904   8.660  1.00  57.25
ATOM   1318  CB   VAL   176    47.638  40.501   8.037  1.00  57.27
ATOM   1319  CG1  VAL   176    48.597  39.511   8.701  1.00  56.21
ATOM   1320  CG2  VAL   176    46.196  40.035   8.199  1.00  56.28
ATOM   1321  C    VAL   176    49.232  42.396   8.362  1.00  57.38
ATOM   1322  O    VAL   176    50.212  41.911   8.926  1.00  57.30
ATOM   1323  N    GLY   177    49.319  43.374   7.467  1.00  57.41
ATOM   1324  CA   GLY   177    50.605  43.939   7.103  1.00  57.60
ATOM   1325  C    GLY   177    51.135  44.878   8.170  1.00  57.50
ATOM   1326  O    GLY   177    52.171  44.605   8.781  1.00  58.09
ATOM   1327  N    LEU   178    50.425  45.982   8.396  1.00  56.68
ATOM   1328  CA   LEU   178    50.837  46.959   9.396  1.00  55.42
ATOM   1329  CB   LEU   178    49.710  47.968   9.646  1.00  55.02
ATOM   1330  CG   LEU   178    49.394  48.906   8.466  1.00  54.15
ATOM   1331  CD1  LEU   178    48.158  49.743   8.766  1.00  53.80
ATOM   1332  CD2  LEU   178    50.588  49.815   8.197  1.00  54.17
ATOM   1333  C    LEU   178    51.247  46.279  10.701  1.00  54.84
ATOM   1334  O    LEU   178    52.177  46.717  11.375  1.00  55.07
ATOM   1335  N    LEU   179    50.575  45.192  11.050  1.00  53.85
ATOM   1336  CA   LEU   179    50.917  44.491  12.274  1.00  53.57
ATOM   1337  CB   LEU   179    49.882  43.409  12.582  1.00  52.75
ATOM   1338  CG   LEU   179    50.099  42.671  13.907  1.00  52.23
ATOM   1339  CD1  LEU   179    49.689  43.580  15.056  1.00  51.63
ATOM   1340  CD2  LEU   179    49.286  41.381  13.935  1.00  51.34
ATOM   1341  C    LEU   179    52.286  43.845  12.128  1.00  54.26
ATOM   1342  O    LEU   179    53.070  43.796  13.075  1.00  54.60
ATOM   1343  N    ARG   180    52.576  43.343  10.932  1.00  54.59
ATOM   1344  CA   ARG   180    53.855  42.679  10.688  1.00  54.08
ATOM   1345  CB   ARG   180    53.824  41.911   9.357  1.00  52.59
ATOM   1346  CG   ARG   180    53.273  40.498   9.515  1.00  50.37
ATOM   1347  CD   ARG   180    53.276  39.702   8.223  1.00  47.24
ATOM   1348  NE   ARG   180    52.610  38.420   8.425  1.00  45.06
ATOM   1349  CZ   ARG   180    51.979  37.754   7.462  1.00  43.97
ATOM   1350  NH1  ARG   180    51.935  38.256   6.226  1.00  42.53
ATOM   1351  NH2  ARG   180    51.366  36.601   7.735  1.00  42.95
ATOM   1352  C    ARG   180    55.059  43.605  10.732  1.00  54.76
ATOM   1353  O    ARG   180    56.009  43.343  11.473  1.00  54.65
ATOM   1354  N    ASP   181    55.036  44.681   9.951  1.00  55.34
ATOM   1355  CA   ASP   181    56.169  45.593   9.972  1.00  56.60
ATOM   1356  CB   ASP   181    56.266  46.386   8.649  1.00  56.43
ATOM   1357  CG   ASP   181    55.132  47.382   8.448  1.00  55.64
ATOM   1358  OD1  ASP   181    54.658  47.483   7.294  1.00  55.20
ATOM   1359  OD2  ASP   181    54.734  48.076   9.416  1.00  55.23
ATOM   1360  C    ASP   181    56.115  46.514  11.199  1.00  57.64
ATOM   1361  O    ASP   181    56.510  47.685  11.153  1.00  57.96
ATOM   1362  N    ALA   182    55.634  45.947  12.303  1.00  57.87
ATOM   1363  CA   ALA   182    55.524  46.646  13.577  1.00  57.84
ATOM   1364  CB   ALA   182    54.078  47.048  13.836  1.00  58.19
```

Figure 4   Sheet 25 of 62

```
ATOM   1365  C    ALA   182      56.013  45.683  14.657  1.00  57.83
ATOM   1366  O    ALA   182      56.681  46.094  15.611  1.00  58.32
ATOM   1367  N    ILE   183      55.669  44.404  14.505  1.00  57.35
ATOM   1368  CA   ILE   183      56.109  43.381  15.448  1.00  57.40
ATOM   1369  CB   ILE   183      55.374  42.036  15.233  1.00  56.09
ATOM   1370  CG2  ILE   183      56.025  40.932  16.074  1.00  55.25
ATOM   1371  CG1  ILE   183      53.904  42.174  15.628  1.00  55.30
ATOM   1372  CD1  ILE   183      53.115  40.881  15.505  1.00  54.14
ATOM   1373  C    ILE   183      57.600  43.164  15.199  1.00  58.51
ATOM   1374  O    ILE   183      58.294  42.531  16.002  1.00  59.24
ATOM   1375  N    LYS   184      58.093  43.689  14.077  1.00  59.04
ATOM   1376  CA   LYS   184      59.508  43.550  13.757  1.00  59.19
ATOM   1377  CB   LYS   184      59.719  43.243  12.268  1.00  59.15
ATOM   1378  CG   LYS   184      59.356  44.354  11.310  1.00  58.36
ATOM   1379  CD   LYS   184      59.566  43.897   9.868  1.00  58.59
ATOM   1380  CE   LYS   184      58.637  42.735   9.500  1.00  59.26
ATOM   1381  NZ   LYS   184      58.751  42.306   8.067  1.00  59.63
ATOM   1382  C    LYS   184      60.270  44.806  14.155  1.00  59.27
ATOM   1383  O    LYS   184      61.382  44.705  14.667  1.00  59.28
ATOM   1384  N    ARG   185      59.695  45.984  13.923  1.00  59.21
ATOM   1385  CA   ARG   185      60.383  47.211  14.331  1.00  59.69
ATOM   1386  CB   ARG   185      59.545  48.458  14.060  1.00  59.70
ATOM   1387  CG   ARG   185      59.278  48.772  12.610  1.00  60.85
ATOM   1388  CD   ARG   185      59.138  50.280  12.443  1.00  60.89
ATOM   1389  NE   ARG   185      58.121  50.628  11.459  1.00  62.26
ATOM   1390  CZ   ARG   185      56.819  50.403  11.620  1.00  61.84
ATOM   1391  NH1  ARG   185      56.372  49.828  12.731  1.00  61.22
ATOM   1392  NH2  ARG   185      55.966  50.754  10.666  1.00  62.23
ATOM   1393  C    ARG   185      60.574  47.104  15.836  1.00  60.41
ATOM   1394  O    ARG   185      61.630  47.430  16.384  1.00  60.45
ATOM   1395  N    ARG   186      59.518  46.633  16.489  1.00  61.07
ATOM   1396  CA   ARG   186      59.489  46.460  17.933  1.00  61.42
ATOM   1397  CB   ARG   186      58.066  46.055  18.358  1.00  61.16
ATOM   1398  CG   ARG   186      57.666  46.433  19.786  1.00  61.08
ATOM   1399  CD   ARG   186      58.249  45.473  20.828  1.00  60.87
ATOM   1400  NE   ARG   186      57.917  45.894  22.188  1.00  61.44
ATOM   1401  CZ   ARG   186      58.294  45.246  23.288  1.00  60.67
ATOM   1402  NH1  ARG   186      59.024  44.133  23.201  1.00  60.28
ATOM   1403  NH2  ARG   186      57.942  45.712  24.481  1.00  61.46
ATOM   1404  C    ARG   186      60.516  45.399  18.344  1.00  61.85
ATOM   1405  O    ARG   186      60.980  44.610  17.514  1.00  62.16
ATOM   1406  N    GLY   187      60.873  45.401  19.628  1.00  62.07
ATOM   1407  CA   GLY   187      61.843  44.455  20.157  1.00  62.22
ATOM   1408  C    GLY   187      61.591  43.017  19.754  1.00  62.50
ATOM   1409  O    GLY   187      60.541  42.692  19.202  1.00  62.37
ATOM   1410  N    ASP   188      62.556  42.148  20.036  1.00  63.08
ATOM   1411  CA   ASP   188      62.414  40.746  19.684  1.00  62.67
ATOM   1412  CB   ASP   188      63.465  39.873  20.373  1.00  61.80
ATOM   1413  CG   ASP   188      63.027  38.409  20.468  1.00  60.64
ATOM   1414  OD1  ASP   188      62.125  38.107  21.289  1.00  60.77
ATOM   1415  OD2  ASP   188      63.565  37.563  19.715  1.00  60.43
ATOM   1416  C    ASP   188      61.047  40.193  20.022  1.00  63.58
ATOM   1417  O    ASP   188      60.441  40.539  21.044  1.00  62.69
ATOM   1418  N    PHE   189      60.599  39.309  19.138  1.00  64.49
ATOM   1419  CA   PHE   189      59.327  38.632  19.249  1.00  64.75
ATOM   1420  CB   PHE   189      58.233  39.629  19.598  1.00  64.84
ATOM   1421  CG   PHE   189      56.886  39.010  19.689  1.00  65.46
```

Figure 4   Sheet 26 of 62

```
ATOM   1422  CD1  PHE   189     56.707  37.824  20.402  1.00  65.54
ATOM   1423  CD2  PHE   189     55.795  39.592  19.052  1.00  65.28
ATOM   1424  CE1  PHE   189     55.455  37.224  20.481  1.00  65.61
ATOM   1425  CE2  PHE   189     54.542  39.007  19.122  1.00  65.71
ATOM   1426  CZ   PHE   189     54.369  37.819  19.839  1.00  65.57
ATOM   1427  C    PHE   189     59.018  37.952  17.919  1.00  65.33
ATOM   1428  O    PHE   189     58.921  38.609  16.881  1.00  64.91
ATOM   1429  N    GLU   190     58.879  36.631  17.956  1.00  66.13
ATOM   1430  CA   GLU   190     58.584  35.854  16.752  1.00  66.57
ATOM   1431  CB   GLU   190     59.387  34.545  16.755  1.00  66.34
ATOM   1432  CG   GLU   190     60.778  34.649  17.389  1.00  64.66
ATOM   1433  CD   GLU   190     61.908  34.356  16.411  1.00  64.02
ATOM   1434  OE1  GLU   190     63.054  34.161  16.874  1.00  63.09
ATOM   1435  OE2  GLU   190     61.658  34.327  15.186  1.00  63.04
ATOM   1436  C    GLU   190     57.093  35.528  16.745  1.00  67.09
ATOM   1437  O    GLU   190     56.609  34.828  17.638  1.00  67.36
ATOM   1438  N    MSE   191     56.367  36.030  15.747  1.00  67.05
ATOM   1439  CA   MSE   191     54.928  35.775  15.666  1.00  66.65
ATOM   1440  CB   MSE   191     54.164  36.920  16.347  1.00  69.47
ATOM   1441  CG   MSE   191     52.867  36.492  17.037  1.00  72.30
ATOM   1442  SE   MSE   191     53.120  35.293  18.409  1.00  78.56
ATOM   1443  CE   MSE   191     51.941  35.893  19.581  1.00  75.88
ATOM   1444  C    MSE   191     54.412  35.590  14.230  1.00  64.85
ATOM   1445  O    MSE   191     54.399  36.538  13.435  1.00  64.30
ATOM   1446  N    ASP   192     53.977  34.368  13.910  1.00  62.82
ATOM   1447  CA   ASP   192     53.449  34.051  12.580  1.00  60.76
ATOM   1448  CB   ASP   192     53.774  32.607  12.207  1.00  61.24
ATOM   1449  CG   ASP   192     55.210  32.427  11.792  1.00  61.76
ATOM   1450  OD1  ASP   192     55.684  33.219  10.947  1.00  62.45
ATOM   1451  OD2  ASP   192     55.863  31.492  12.299  1.00  62.32
ATOM   1452  C    ASP   192     51.942  34.266  12.459  1.00  59.03
ATOM   1453  O    ASP   192     51.143  33.375  12.767  1.00  58.37
ATOM   1454  N    VAL   193     51.567  35.453  11.991  1.00  57.00
ATOM   1455  CA   VAL   193     50.167  35.818  11.818  1.00  54.85
ATOM   1456  CB   VAL   193     50.034  37.305  11.454  1.00  55.09
ATOM   1457  CG1  VAL   193     48.568  37.712  11.448  1.00  54.84
ATOM   1458  CG2  VAL   193     50.826  38.146  12.441  1.00  54.87
ATOM   1459  C    VAL   193     49.473  34.977  10.746  1.00  53.19
ATOM   1460  O    VAL   193     49.500  35.303   9.555  1.00  52.03
ATOM   1461  N    VAL   194     48.854  33.894  11.205  1.00  51.82
ATOM   1462  CA   VAL   194     48.126  32.949  10.367  1.00  50.66
ATOM   1463  CB   VAL   194     47.841  31.644  11.174  1.00  51.08
ATOM   1464  CG1  VAL   194     46.686  30.860  10.554  1.00  52.09
ATOM   1465  CG2  VAL   194     49.091  30.778  11.211  1.00  51.33
ATOM   1466  C    VAL   194     46.798  33.498   9.808  1.00  49.99
ATOM   1467  O    VAL   194     46.677  33.726   8.602  1.00  49.40
ATOM   1468  N    ALA   195     45.813  33.723  10.683  1.00  48.93
ATOM   1469  CA   ALA   195     44.499  34.193  10.251  1.00  47.60
ATOM   1470  CB   ALA   195     43.467  33.123  10.572  1.00  47.58
ATOM   1471  C    ALA   195     43.992  35.546  10.760  1.00  46.68
ATOM   1472  O    ALA   195     44.344  35.996  11.851  1.00  46.16
ATOM   1473  N    MSE   196     43.157  36.182   9.940  1.00  45.43
ATOM   1474  CA   MSE   196     42.521  37.459  10.279  1.00  44.60
ATOM   1475  CB   MSE   196     43.079  38.623   9.451  1.00  45.32
ATOM   1476  CG   MSE   196     42.329  39.925   9.716  1.00  47.29
ATOM   1477  SE   MSE   196     42.937  41.426   8.852  1.00  53.21
ATOM   1478  CE   MSE   196     44.264  41.920   9.982  1.00  51.44
```

Figure 4   Sheet 27 of 62

ATOM	1479	C	MSE	196	41.019	37.333	10.002	1.00	43.09
ATOM	1480	O	MSE	196	40.610	36.973	8.892	1.00	43.71
ATOM	1481	N	VAL	197	40.190	37.631	10.996	1.00	40.47
ATOM	1482	CA	VAL	197	38.751	37.514	10.799	1.00	37.00
ATOM	1483	CB	VAL	197	38.240	36.228	11.458	1.00	37.31
ATOM	1484	CG1	VAL	197	38.840	35.004	10.766	1.00	36.64
ATOM	1485	CG2	VAL	197	38.643	36.217	12.914	1.00	36.88
ATOM	1486	C	VAL	197	37.991	38.710	11.354	1.00	35.22
ATOM	1487	O	VAL	197	38.561	39.544	12.057	1.00	35.21
ATOM	1488	N	ASN	198	36.708	38.801	11.015	1.00	33.39
ATOM	1489	CA	ASN	198	35.830	39.883	11.491	1.00	30.23
ATOM	1490	CB	ASN	198	34.740	40.175	10.446	1.00	30.65
ATOM	1491	CG	ASN	198	33.801	41.309	10.852	1.00	31.35
ATOM	1492	OD1	ASN	198	32.907	41.128	11.686	1.00	32.70
ATOM	1493	ND2	ASN	198	33.997	42.486	10.251	1.00	30.53
ATOM	1494	C	ASN	198	35.217	39.356	12.780	1.00	28.41
ATOM	1495	O	ASN	198	35.052	38.143	12.937	1.00	26.14
ATOM	1496	N	ASP	199	34.892	40.252	13.711	1.00	27.77
ATOM	1497	CA	ASP	199	34.325	39.816	14.990	1.00	26.87
ATOM	1498	CB	ASP	199	34.156	41.007	15.945	1.00	26.75
ATOM	1499	CG	ASP	199	33.254	42.097	15.396	1.00	26.24
ATOM	1500	OD1	ASP	199	33.221	42.292	14.167	1.00	26.90
ATOM	1501	OD2	ASP	199	32.587	42.777	16.205	1.00	26.19
ATOM	1502	C	ASP	199	33.027	39.034	14.843	1.00	26.43
ATOM	1503	O	ASP	199	32.715	38.188	15.684	1.00	27.02
ATOM	1504	N	THR	200	32.291	39.292	13.763	1.00	25.45
ATOM	1505	CA	THR	200	31.050	38.585	13.510	1.00	25.65
ATOM	1506	CB	THR	200	30.261	39.193	12.339	1.00	25.75
ATOM	1507	OG1	THR	200	31.008	39.044	11.130	1.00	26.04
ATOM	1508	CG2	THR	200	30.002	40.672	12.573	1.00	26.48
ATOM	1509	C	THR	200	31.383	37.155	13.143	1.00	26.96
ATOM	1510	O	THR	200	30.832	36.211	13.712	1.00	27.62
ATOM	1511	N	VAL	201	32.295	36.990	12.189	1.00	28.07
ATOM	1512	CA	VAL	201	32.695	35.654	11.742	1.00	28.50
ATOM	1513	CB	VAL	201	33.785	35.726	10.665	1.00	29.26
ATOM	1514	CG1	VAL	201	34.056	34.332	10.123	1.00	31.22
ATOM	1515	CG2	VAL	201	33.370	36.684	9.546	1.00	27.90
ATOM	1516	C	VAL	201	33.231	34.818	12.901	1.00	29.16
ATOM	1517	O	VAL	201	32.816	33.676	13.101	1.00	29.44
ATOM	1518	N	ALA	202	34.156	35.395	13.663	1.00	30.31
ATOM	1519	CA	ALA	202	34.752	34.710	14.812	1.00	32.23
ATOM	1520	CB	ALA	202	35.591	35.705	15.643	1.00	31.72
ATOM	1521	C	ALA	202	33.688	34.070	15.696	1.00	33.37
ATOM	1522	O	ALA	202	33.789	32.894	16.073	1.00	34.14
ATOM	1523	N	THR	203	32.667	34.858	16.019	1.00	34.41
ATOM	1524	CA	THR	203	31.566	34.422	16.870	1.00	35.37
ATOM	1525	CB	THR	203	30.614	35.604	17.117	1.00	36.27
ATOM	1526	OG1	THR	203	31.370	36.708	17.645	1.00	37.04
ATOM	1527	CG2	THR	203	29.500	35.213	18.090	1.00	35.19
ATOM	1528	C	THR	203	30.800	33.260	16.242	1.00	36.08
ATOM	1529	O	THR	203	30.538	32.241	16.891	1.00	35.34
ATOM	1530	N	MSE	204	30.433	33.415	14.978	1.00	36.89
ATOM	1531	CA	MSE	204	29.722	32.348	14.299	1.00	37.94
ATOM	1532	CB	MSE	204	29.582	32.665	12.811	1.00	39.76
ATOM	1533	CG	MSE	204	29.065	31.504	11.954	1.00	40.74
ATOM	1534	SE	MSE	204	29.135	31.967	10.181	1.00	45.75
ATOM	1535	CE	MSE	204	30.643	31.057	9.627	1.00	45.26

Figure 4   Sheet 28 of 62

```
ATOM   1536   C    MSE   204      30.531   31.075   14.465   1.00   38.36
ATOM   1537   O    MSE   204      30.024   30.064   14.954   1.00   37.86
ATOM   1538   N    ILE   205      31.798   31.148   14.061   1.00   38.79
ATOM   1539   CA   ILE   205      32.696   30.008   14.137   1.00   40.09
ATOM   1540   CB   ILE   205      34.178   30.451   13.981   1.00   39.81
ATOM   1541   CG2  ILE   205      35.098   29.240   14.072   1.00   39.47
ATOM   1542   CG1  ILE   205      34.398   31.112   12.616   1.00   39.46
ATOM   1543   CD1  ILE   205      34.250   30.158   11.425   1.00   39.34
ATOM   1544   C    ILE   205      32.527   29.215   15.440   1.00   41.34
ATOM   1545   O    ILE   205      32.121   28.050   15.408   1.00   41.41
ATOM   1546   N    SER   206      32.812   29.830   16.584   1.00   42.01
ATOM   1547   CA   SER   206      32.683   29.112   17.849   1.00   43.71
ATOM   1548   CB   SER   206      32.999   30.038   19.013   1.00   43.57
ATOM   1549   OG   SER   206      32.149   31.163   18.971   1.00   44.54
ATOM   1550   C    SER   206      31.306   28.494   18.056   1.00   44.83
ATOM   1551   O    SER   206      31.185   27.304   18.364   1.00   45.40
ATOM   1552   N    CYS   207      30.260   29.291   17.894   1.00   46.32
ATOM   1553   CA   CYS   207      28.912   28.764   18.079   1.00   48.14
ATOM   1554   CB   CYS   207      27.869   29.842   17.780   1.00   46.74
ATOM   1555   SG   CYS   207      27.946   31.264   18.883   1.00   42.50
ATOM   1556   C    CYS   207      28.666   27.551   17.186   1.00   50.79
ATOM   1557   O    CYS   207      27.715   26.799   17.403   1.00   50.97
ATOM   1558   N    TYR   208      29.533   27.361   16.190   1.00   53.91
ATOM   1559   CA   TYR   208      29.418   26.243   15.247   1.00   56.61
ATOM   1560   CB   TYR   208      30.350   26.458   14.045   1.00   56.96
ATOM   1561   CG   TYR   208      30.370   25.303   13.062   1.00   57.29
ATOM   1562   CD1  TYR   208      29.307   25.090   12.182   1.00   57.54
ATOM   1563   CE1  TYR   208      29.319   24.026   11.280   1.00   57.47
ATOM   1564   CD2  TYR   208      31.448   24.418   13.019   1.00   57.54
ATOM   1565   CE2  TYR   208      31.468   23.350   12.125   1.00   57.60
ATOM   1566   CZ   TYR   208      30.404   23.163   11.258   1.00   57.47
ATOM   1567   OH   TYR   208      30.435   22.126   10.360   1.00   57.71
ATOM   1568   C    TYR   208      29.705   24.867   15.854   1.00   58.12
ATOM   1569   O    TYR   208      28.874   23.960   15.773   1.00   58.61
ATOM   1570   N    TYR   209      30.876   24.699   16.459   1.00   59.77
ATOM   1571   CA   TYR   209      31.198   23.399   17.028   1.00   61.36
ATOM   1572   CB   TYR   209      32.619   23.394   17.581   1.00   63.23
ATOM   1573   CG   TYR   209      33.648   23.401   16.472   1.00   65.26
ATOM   1574   CD1  TYR   209      34.058   24.595   15.876   1.00   66.13
ATOM   1575   CE1  TYR   209      34.959   24.594   14.807   1.00   67.31
ATOM   1576   CD2  TYR   209      34.165   22.206   15.973   1.00   65.88
ATOM   1577   CE2  TYR   209      35.062   22.193   14.906   1.00   66.79
ATOM   1578   CZ   TYR   209      35.457   23.386   14.328   1.00   67.37
ATOM   1579   OH   TYR   209      36.350   23.370   13.277   1.00   67.62
ATOM   1580   C    TYR   209      30.206   22.965   18.083   1.00   61.32
ATOM   1581   O    TYR   209      30.048   21.771   18.336   1.00   61.19
ATOM   1582   N    GLU   210      29.523   23.938   18.680   1.00   61.63
ATOM   1583   CA   GLU   210      28.524   23.658   19.701   1.00   61.05
ATOM   1584   CB   GLU   210      28.444   24.808   20.706   1.00   62.29
ATOM   1585   CG   GLU   210      27.539   24.499   21.884   1.00   65.45
ATOM   1586   CD   GLU   210      27.716   25.463   23.050   1.00   67.38
ATOM   1587   OE1  GLU   210      28.865   25.609   23.535   1.00   68.93
ATOM   1588   OE2  GLU   210      26.707   26.065   23.488   1.00   67.92
ATOM   1589   C    GLU   210      27.175   23.459   19.026   1.00   60.04
ATOM   1590   O    GLU   210      26.255   22.901   19.618   1.00   59.93
ATOM   1591   N    ASP   211      27.073   23.920   17.780   1.00   58.82
ATOM   1592   CA   ASP   211      25.849   23.797   16.984   1.00   57.80
```

```
ATOM    1593  CB   ASP   211      24.804  24.824  17.441  1.00  58.16
ATOM    1594  CG   ASP   211      23.504  24.730  16.653  1.00  58.25
ATOM    1595  OD1  ASP   211      22.490  25.299  17.111  1.00  57.88
ATOM    1596  OD2  ASP   211      23.495  24.096  15.572  1.00  58.65
ATOM    1597  C    ASP   211      26.173  23.993  15.503  1.00  56.54
ATOM    1598  O    ASP   211      26.351  25.116  15.037  1.00  56.17
ATOM    1599  N    HIS   212      26.234  22.884  14.773  1.00  55.81
ATOM    1600  CA   HIS   212      26.577  22.884  13.351  1.00  55.26
ATOM    1601  CB   HIS   212      26.699  21.442  12.852  1.00  57.87
ATOM    1602  CG   HIS   212      27.816  20.678  13.493  1.00  61.52
ATOM    1603  CD2  HIS   212      27.815  19.527  14.205  1.00  62.63
ATOM    1604  ND1  HIS   212      29.127  21.110  13.460  1.00  62.80
ATOM    1605  CE1  HIS   212      29.884  20.258  14.127  1.00  63.70
ATOM    1606  NE2  HIS   212      29.114  19.288  14.590  1.00  63.71
ATOM    1607  C    HIS   212      25.665  23.656  12.412  1.00  53.29
ATOM    1608  O    HIS   212      26.014  23.883  11.251  1.00  52.77
ATOM    1609  N    GLN   213      24.496  24.058  12.895  1.00  51.08
ATOM    1610  CA   GLN   213      23.579  24.790  12.037  1.00  48.22
ATOM    1611  CB   GLN   213      22.135  24.347  12.298  1.00  49.39
ATOM    1612  CG   GLN   213      21.957  22.839  12.130  1.00  50.76
ATOM    1613  CD   GLN   213      20.507  22.410  11.965  1.00  51.82
ATOM    1614  OE1  GLN   213      19.653  22.721  12.803  1.00  52.48
ATOM    1615  NE2  GLN   213      20.223  21.679  10.883  1.00  51.72
ATOM    1616  C    GLN   213      23.746  26.289  12.202  1.00  45.19
ATOM    1617  O    GLN   213      22.978  27.077  11.654  1.00  45.00
ATOM    1618  N    CYS   214      24.759  26.686  12.957  1.00  41.87
ATOM    1619  CA   CYS   214      25.015  28.105  13.122  1.00  39.08
ATOM    1620  CB   CYS   214      25.907  28.386  14.332  1.00  39.18
ATOM    1621  SG   CYS   214      26.281  30.175  14.542  1.00  40.32
ATOM    1622  C    CYS   214      25.743  28.530  11.859  1.00  36.43
ATOM    1623  O    CYS   214      26.915  28.214  11.689  1.00  36.06
ATOM    1624  N    GLU   215      25.046  29.223  10.967  1.00  33.00
ATOM    1625  CA   GLU   215      25.664  29.672   9.736  1.00  30.60
ATOM    1626  CB   GLU   215      25.056  28.960   8.541  1.00  31.95
ATOM    1627  CG   GLU   215      25.289  27.466   8.561  1.00  33.57
ATOM    1628  CD   GLU   215      24.973  26.827   7.233  1.00  35.80
ATOM    1629  OE1  GLU   215      25.719  27.094   6.264  1.00  37.32
ATOM    1630  OE2  GLU   215      23.978  26.064   7.156  1.00  37.21
ATOM    1631  C    GLU   215      25.518  31.162   9.563  1.00  28.84
ATOM    1632  O    GLU   215      25.665  31.687   8.459  1.00  28.39
ATOM    1633  N    VAL   216      25.243  31.847  10.669  1.00  26.45
ATOM    1634  CA   VAL   216      25.083  33.291  10.648  1.00  23.67
ATOM    1635  CB   VAL   216      23.589  33.706  10.607  1.00  23.44
ATOM    1636  CG1  VAL   216      23.485  35.214  10.492  1.00  22.72
ATOM    1637  CG2  VAL   216      22.875  33.031   9.449  1.00  22.30
ATOM    1638  C    VAL   216      25.671  33.858  11.921  1.00  22.20
ATOM    1639  O    VAL   216      25.444  33.328  13.006  1.00  22.86
ATOM    1640  N    GLY   217      26.423  34.939  11.793  1.00  21.40
ATOM    1641  CA   GLY   217      26.997  35.554  12.965  1.00  21.14
ATOM    1642  C    GLY   217      26.524  36.994  13.022  1.00  22.30
ATOM    1643  O    GLY   217      26.432  37.677  11.983  1.00  22.05
ATOM    1644  N    MSE   218      26.201  37.454  14.228  1.00  23.03
ATOM    1645  CA   MSE   218      25.748  38.815  14.414  1.00  23.03
ATOM    1646  CB   MSE   218      24.208  38.880  14.445  1.00  25.98
ATOM    1647  CG   MSE   218      23.647  40.306  14.646  1.00  28.99
ATOM    1648  SE   MSE   218      21.806  40.486  14.543  1.00  35.34
ATOM    1649  CE   MSE   218      21.273  39.804  16.207  1.00  31.95
```

Figure 4   Sheet 30 of 62

```
ATOM   1650  C    MSE   218      26.320  39.405  15.694  1.00  21.99
ATOM   1651  O    MSE   218      26.425  38.738  16.724  1.00  22.34
ATOM   1652  N    ILE   219      26.694  40.670  15.606  1.00  21.28
ATOM   1653  CA   ILE   219      27.240  41.402  16.720  1.00  20.85
ATOM   1654  CB   ILE   219      28.702  41.840  16.449  1.00  20.74
ATOM   1655  CG2  ILE   219      29.164  42.757  17.558  1.00  19.65
ATOM   1656  CG1  ILE   219      29.623  40.627  16.335  1.00  19.32
ATOM   1657  CD1  ILE   219      29.656  39.770  17.596  1.00  20.63
ATOM   1658  C    ILE   219      26.413  42.676  16.838  1.00  21.47
ATOM   1659  O    ILE   219      26.297  43.431  15.868  1.00  21.30
ATOM   1660  N    VAL   220      25.823  42.908  18.003  1.00  21.91
ATOM   1661  CA   VAL   220      25.059  44.135  18.224  1.00  22.49
ATOM   1662  CB   VAL   220      23.563  43.873  18.479  1.00  22.04
ATOM   1663  CG1  VAL   220      22.815  45.183  18.425  1.00  21.50
ATOM   1664  CG2  VAL   220      23.007  42.901  17.463  1.00  22.03
ATOM   1665  C    VAL   220      25.650  44.775  19.477  1.00  23.27
ATOM   1666  O    VAL   220      25.095  44.642  20.575  1.00  23.94
ATOM   1667  N    GLY   221      26.795  45.436  19.312  1.00  22.78
ATOM   1668  CA   GLY   221      27.448  46.063  20.443  1.00  22.86
ATOM   1669  C    GLY   221      27.728  47.509  20.138  1.00  23.75
ATOM   1670  O    GLY   221      26.816  48.264  19.828  1.00  25.09
ATOM   1671  N    THR   222      28.988  47.906  20.233  1.00  24.06
ATOM   1672  CA   THR   222      29.375  49.277  19.939  1.00  24.06
ATOM   1673  CB   THR   222      30.893  49.423  19.960  1.00  24.59
ATOM   1674  OG1  THR   222      31.377  49.051  21.258  1.00  26.00
ATOM   1675  CG2  THR   222      31.299  50.860  19.640  1.00  24.67
ATOM   1676  C    THR   222      28.888  49.530  18.533  1.00  24.09
ATOM   1677  O    THR   222      28.248  50.530  18.259  1.00  24.72
ATOM   1678  N    GLY   223      29.211  48.597  17.646  1.00  24.40
ATOM   1679  CA   GLY   223      28.790  48.686  16.262  1.00  24.65
ATOM   1680  C    GLY   223      27.797  47.560  16.020  1.00  25.05
ATOM   1681  O    GLY   223      27.478  46.779  16.936  1.00  25.80
ATOM   1682  N    CYS   224      27.298  47.453  14.798  1.00  24.73
ATOM   1683  CA   CYS   224      26.338  46.405  14.504  1.00  24.18
ATOM   1684  CB   CYS   224      24.928  46.958  14.682  1.00  24.47
ATOM   1685  SG   CYS   224      23.640  45.925  13.998  1.00  25.11
ATOM   1686  C    CYS   224      26.550  45.895  13.085  1.00  23.65
ATOM   1687  O    CYS   224      26.618  46.683  12.144  1.00  24.07
ATOM   1688  N    ASN   225      26.650  44.578  12.941  1.00  23.06
ATOM   1689  CA   ASN   225      26.883  43.963  11.638  1.00  23.27
ATOM   1690  CB   ASN   225      28.346  44.230  11.210  1.00  26.15
ATOM   1691  CG   ASN   225      28.831  43.296  10.098  1.00  27.94
ATOM   1692  OD1  ASN   225      28.271  43.265   8.997  1.00  29.23
ATOM   1693  ND2  ASN   225      29.878  42.524  10.393  1.00  28.62
ATOM   1694  C    ASN   225      26.603  42.459  11.740  1.00  21.80
ATOM   1695  O    ASN   225      26.291  41.954  12.827  1.00  20.54
ATOM   1696  N    ALA   226      26.709  41.759  10.610  1.00  19.99
ATOM   1697  CA   ALA   226      26.478  40.322  10.566  1.00  19.47
ATOM   1698  CB   ALA   226      24.994  40.032  10.443  1.00  20.99
ATOM   1699  C    ALA   226      27.194  39.723   9.378  1.00  18.72
ATOM   1700  O    ALA   226      27.529  40.428   8.415  1.00  17.97
ATOM   1701  N    CYS   227      27.404  38.415   9.439  1.00  18.36
ATOM   1702  CA   CYS   227      28.077  37.675   8.368  1.00  19.35
ATOM   1703  CB   CYS   227      29.523  37.396   8.751  1.00  18.42
ATOM   1704  SG   CYS   227      29.556  36.326  10.207  1.00  20.13
ATOM   1705  C    CYS   227      27.331  36.352   8.291  1.00  19.81
ATOM   1706  O    CYS   227      26.702  35.951   9.280  1.00  20.62
```

Figure 4   Sheet 31 of 62

ATOM	1707	N	TYR	228	27.402	35.668	7.148	1.00	20.49
ATOM	1708	CA	TYR	228	26.705	34.384	6.989	1.00	20.56
ATOM	1709	CB	TYR	228	25.242	34.633	6.624	1.00	17.90
ATOM	1710	CG	TYR	228	25.096	35.134	5.204	1.00	15.65
ATOM	1711	CD1	TYR	228	24.922	34.249	4.145	1.00	15.81
ATOM	1712	CE1	TYR	228	24.885	34.701	2.823	1.00	15.89
ATOM	1713	CD2	TYR	228	25.221	36.483	4.913	1.00	15.28
ATOM	1714	CE2	TYR	228	25.186	36.949	3.601	1.00	16.08
ATOM	1715	CZ	TYR	228	25.022	36.051	2.564	1.00	16.76
ATOM	1716	OH	TYR	228	25.033	36.505	1.263	1.00	18.93
ATOM	1717	C	TYR	228	27.345	33.539	5.887	1.00	22.19
ATOM	1718	O	TYR	228	28.174	34.024	5.112	1.00	21.49
ATOM	1719	N	MSE	229	26.928	32.278	5.808	1.00	24.74
ATOM	1720	CA	MSE	229	27.438	31.349	4.808	1.00	26.69
ATOM	1721	CB	MSE	229	27.342	29.918	5.339	1.00	28.61
ATOM	1722	CG	MSE	229	28.167	29.637	6.598	1.00	32.37
ATOM	1723	SE	MSE	229	29.987	30.056	6.460	1.00	41.17
ATOM	1724	CE	MSE	229	30.544	28.874	5.098	1.00	36.30
ATOM	1725	C	MSE	229	26.663	31.470	3.481	1.00	27.83
ATOM	1726	O	MSE	229	25.535	30.994	3.363	1.00	28.02
ATOM	1727	N	GLU	230	27.282	32.109	2.492	1.00	29.19
ATOM	1728	CA	GLU	230	26.688	32.296	1.172	1.00	29.81
ATOM	1729	CB	GLU	230	27.165	33.623	0.577	1.00	30.83
ATOM	1730	CG	GLU	230	26.685	33.922	-0.843	1.00	32.33
ATOM	1731	CD	GLU	230	25.173	33.825	-0.989	1.00	34.04
ATOM	1732	OE1	GLU	230	24.663	32.698	-1.222	1.00	34.43
ATOM	1733	OE2	GLU	230	24.497	34.878	-0.858	1.00	33.65
ATOM	1734	C	GLU	230	27.127	31.143	0.282	1.00	30.91
ATOM	1735	O	GLU	230	27.958	30.319	0.685	1.00	30.80
ATOM	1736	N	GLU	231	26.562	31.078	-0.923	1.00	32.47
ATOM	1737	CA	GLU	231	26.885	30.024	-1.883	1.00	34.04
ATOM	1738	CB	GLU	231	25.668	29.696	-2.745	1.00	34.21
ATOM	1739	CG	GLU	231	24.408	29.396	-1.979	1.00	34.89
ATOM	1740	CD	GLU	231	24.452	28.054	-1.296	1.00	36.36
ATOM	1741	OE1	GLU	231	24.745	27.064	-2.002	1.00	36.80
ATOM	1742	OE2	GLU	231	24.182	27.981	-0.067	1.00	36.72
ATOM	1743	C	GLU	231	27.997	30.550	-2.777	1.00	35.65
ATOM	1744	O	GLU	231	27.889	31.663	-3.304	1.00	35.42
ATOM	1745	N	MSE	232	29.060	29.758	-2.952	1.00	37.13
ATOM	1746	CA	MSE	232	30.188	30.181	-3.780	1.00	38.19
ATOM	1747	CB	MSE	232	31.191	29.036	-3.935	1.00	41.27
ATOM	1748	CG	MSE	232	32.195	28.912	-2.765	1.00	45.40
ATOM	1749	SE	MSE	232	33.237	30.431	-2.467	1.00	52.07
ATOM	1750	CE	MSE	232	34.286	30.483	-3.969	1.00	48.20
ATOM	1751	C	MSE	232	29.694	30.664	-5.137	1.00	38.02
ATOM	1752	O	MSE	232	30.179	31.656	-5.678	1.00	36.84
ATOM	1753	N	GLN	233	28.698	29.970	-5.668	1.00	38.35
ATOM	1754	CA	GLN	233	28.110	30.331	-6.948	1.00	38.79
ATOM	1755	CB	GLN	233	26.954	29.373	-7.257	1.00	40.19
ATOM	1756	CG	GLN	233	25.658	30.041	-7.672	1.00	41.80
ATOM	1757	CD	GLN	233	24.460	29.119	-7.510	1.00	43.22
ATOM	1758	OE1	GLN	233	24.226	28.582	-6.424	1.00	44.27
ATOM	1759	NE2	GLN	233	23.688	28.936	-8.586	1.00	43.87
ATOM	1760	C	GLN	233	27.615	31.777	-6.936	1.00	38.45
ATOM	1761	O	GLN	233	27.495	32.407	-7.984	1.00	39.07
ATOM	1762	N	ASN	234	27.329	32.313	-5.753	1.00	37.79
ATOM	1763	CA	ASN	234	26.840	33.687	-5.668	1.00	36.56

Figure 4 Sheet 32 of 62

```
ATOM   1764  CB  ASN  234   25.657  33.771  -4.706  1.00  37.03
ATOM   1765  CG  ASN  234   24.505  32.864  -5.119  1.00  36.83
ATOM   1766  OD1 ASN  234   24.152  32.793  -6.299  1.00  36.50
ATOM   1767  ND2 ASN  234   23.910  32.173  -4.146  1.00  36.25
ATOM   1768  C   ASN  234   27.919  34.676  -5.250  1.00  35.71
ATOM   1769  O   ASN  234   27.712  35.890  -5.301  1.00  35.11
ATOM   1770  N   VAL  235   29.069  34.156  -4.837  1.00  35.22
ATOM   1771  CA  VAL  235   30.177  35.009  -4.439  1.00  34.85
ATOM   1772  CB  VAL  235   31.056  34.321  -3.384  1.00  34.01
ATOM   1773  CG1 VAL  235   31.949  35.343  -2.717  1.00  32.35
ATOM   1774  CG2 VAL  235   30.185  33.576  -2.376  1.00  32.63
ATOM   1775  C   VAL  235   30.999  35.209  -5.706  1.00  35.79
ATOM   1776  O   VAL  235   32.011  34.548  -5.910  1.00  35.65
ATOM   1777  N   GLU  236   30.556  36.125  -6.556  1.00  37.55
ATOM   1778  CA  GLU  236   31.220  36.383  -7.830  1.00  39.52
ATOM   1779  CB  GLU  236   30.337  37.284  -8.701  1.00  39.67
ATOM   1780  CG  GLU  236   29.242  36.539  -9.448  1.00  41.02
ATOM   1781  CD  GLU  236   28.214  37.467 -10.072  1.00  42.58
ATOM   1782  OE1 GLU  236   28.607  38.529 -10.630  1.00  42.67
ATOM   1783  OE2 GLU  236   27.009  37.121 -10.011  1.00  43.02
ATOM   1784  C   GLU  236   32.631  36.961  -7.782  1.00  40.97
ATOM   1785  O   GLU  236   33.328  36.967  -8.803  1.00  42.27
ATOM   1786  N   LEU  237   33.064  37.457  -6.628  1.00  41.32
ATOM   1787  CA  LEU  237   34.408  38.017  -6.538  1.00  41.63
ATOM   1788  CB  LEU  237   34.438  39.163  -5.537  1.00  41.68
ATOM   1789  CG  LEU  237   33.545  40.367  -5.820  1.00  42.50
ATOM   1790  CD1 LEU  237   33.630  41.301  -4.623  1.00  44.17
ATOM   1791  CD2 LEU  237   33.984  41.101  -7.085  1.00  42.46
ATOM   1792  C   LEU  237   35.454  36.970  -6.148  1.00  42.43
ATOM   1793  O   LEU  237   36.636  37.294  -6.010  1.00  42.30
ATOM   1794  N   VAL  238   35.019  35.724  -5.967  1.00  42.96
ATOM   1795  CA  VAL  238   35.922  34.629  -5.606  1.00  43.89
ATOM   1796  CB  VAL  238   35.917  34.380  -4.097  1.00  42.33
ATOM   1797  CG1 VAL  238   36.722  33.136  -3.769  1.00  41.32
ATOM   1798  CG2 VAL  238   36.503  35.578  -3.385  1.00  42.74
ATOM   1799  C   VAL  238   35.520  33.337  -6.313  1.00  45.65
ATOM   1800  O   VAL  238   34.755  32.555  -5.770  1.00  46.15
ATOM   1801  N   GLU  239   36.069  33.116  -7.510  1.00  47.60
ATOM   1802  CA  GLU  239   35.769  31.947  -8.346  1.00  48.96
ATOM   1803  CB  GLU  239   36.819  31.793  -9.448  1.00  51.17
ATOM   1804  CG  GLU  239   37.000  33.026 -10.290  1.00  53.95
ATOM   1805  CD  GLU  239   37.817  34.066  -9.570  1.00  56.27
ATOM   1806  OE1 GLU  239   39.070  33.982  -9.637  1.00  58.40
ATOM   1807  OE2 GLU  239   37.211  34.950  -8.918  1.00  57.25
ATOM   1808  C   GLU  239   35.599  30.594  -7.675  1.00  48.87
ATOM   1809  O   GLU  239   36.272  30.274  -6.701  1.00  48.25
ATOM   1810  N   GLY  240   34.705  29.797  -8.252  1.00  49.09
ATOM   1811  CA  GLY  240   34.412  28.469  -7.750  1.00  50.05
ATOM   1812  C   GLY  240   32.967  28.418  -7.296  1.00  51.04
ATOM   1813  O   GLY  240   32.482  29.379  -6.712  1.00  52.00
ATOM   1814  N   ASP  241   32.259  27.332  -7.580  1.00  51.38
ATOM   1815  CA  ASP  241   30.882  27.214  -7.127  1.00  52.10
ATOM   1816  CB  ASP  241   29.963  26.766  -8.252  1.00  52.95
ATOM   1817  CG  ASP  241   30.186  27.534  -9.529  1.00  53.84
ATOM   1818  OD1 ASP  241   30.046  28.779  -9.522  1.00  53.20
ATOM   1819  OD2 ASP  241   30.496  26.875 -10.546  1.00  53.97
ATOM   1820  C   ASP  241   30.924  26.122  -6.083  1.00  52.90
```

Figure 4   Sheet 33 of 62

```
ATOM   1821   O     ASP   241     29.898   25.563   -5.701   1.00   53.59
ATOM   1822   N     GLU   242     32.131   25.816   -5.626   1.00   53.45
ATOM   1823   CA    GLU   242     32.325   24.760   -4.646   1.00   53.65
ATOM   1824   CB    GLU   242     33.785   24.299   -4.670   1.00   55.19
ATOM   1825   CG    GLU   242     34.056   23.062   -3.826   1.00   57.57
ATOM   1826   CD    GLU   242     35.527   22.672   -3.811   1.00   58.85
ATOM   1827   OE1   GLU   242     36.063   22.340   -4.893   1.00   59.63
ATOM   1828   OE2   GLU   242     36.143   22.701   -2.717   1.00   59.85
ATOM   1829   C     GLU   242     31.933   25.159   -3.229   1.00   52.66
ATOM   1830   O     GLU   242     32.469   26.113   -2.661   1.00   53.15
ATOM   1831   N     GLY   243     30.987   24.418   -2.665   1.00   51.11
ATOM   1832   CA    GLY   243     30.545   24.673   -1.305   1.00   48.74
ATOM   1833   C     GLY   243     30.200   26.110   -0.967   1.00   46.87
ATOM   1834   O     GLY   243     29.879   26.917   -1.850   1.00   46.49
ATOM   1835   N     ARG   244     30.288   26.421    0.326   1.00   44.89
ATOM   1836   CA    ARG   244     29.967   27.748    0.838   1.00   43.27
ATOM   1837   CB    ARG   244     28.852   27.639    1.873   1.00   42.24
ATOM   1838   CG    ARG   244     27.571   27.040    1.339   1.00   42.16
ATOM   1839   CD    ARG   244     26.442   27.153    2.356   1.00   41.35
ATOM   1840   NE    ARG   244     25.254   26.425    1.925   1.00   39.30
ATOM   1841   CZ    ARG   244     24.702   25.446    2.630   1.00   39.15
ATOM   1842   NH1   ARG   244     25.236   25.085    3.794   1.00   38.10
ATOM   1843   NH2   ARG   244     23.627   24.821    2.168   1.00   38.77
ATOM   1844   C     ARG   244     31.121   28.524    1.465   1.00   42.34
ATOM   1845   O     ARG   244     32.089   27.945    1.958   1.00   41.77
ATOM   1846   N     MSE   245     30.990   29.849    1.446   1.00   42.07
ATOM   1847   CA    MSE   245     31.977   30.745    2.042   1.00   41.32
ATOM   1848   CB    MSE   245     32.846   31.391    0.974   1.00   42.25
ATOM   1849   CG    MSE   245     33.870   32.345    1.566   1.00   44.07
ATOM   1850   SE    MSE   245     34.884   33.206    0.332   1.00   47.16
ATOM   1851   CE    MSE   245     36.149   31.909   -0.005   1.00   44.40
ATOM   1852   C     MSE   245     31.324   31.863    2.863   1.00   40.37
ATOM   1853   O     MSE   245     30.525   32.644    2.338   1.00   40.13
ATOM   1854   N     CYS   246     31.664   31.940    4.148   1.00   38.95
ATOM   1855   CA    CYS   246     31.125   32.990    5.001   1.00   37.00
ATOM   1856   CB    CYS   246     31.794   32.953    6.376   1.00   37.69
ATOM   1857   SG    CYS   246     31.231   34.229    7.567   1.00   38.96
ATOM   1858   C     CYS   246     31.422   34.320    4.311   1.00   35.82
ATOM   1859   O     CYS   246     32.484   34.497    3.706   1.00   34.54
ATOM   1860   N     VAL   247     30.466   35.240    4.388   1.00   34.51
ATOM   1861   CA    VAL   247     30.591   36.566    3.782   1.00   32.46
ATOM   1862   CB    VAL   247     29.609   36.751    2.588   1.00   32.34
ATOM   1863   CG1   VAL   247     29.709   38.170    2.038   1.00   31.78
ATOM   1864   CG2   VAL   247     29.930   35.750    1.486   1.00   32.04
ATOM   1865   C     VAL   247     30.239   37.580    4.863   1.00   32.03
ATOM   1866   O     VAL   247     29.291   37.377    5.628   1.00   33.28
ATOM   1867   N     ASN   248     31.011   38.657    4.931   1.00   29.34
ATOM   1868   CA    ASN   248     30.792   39.699    5.917   1.00   27.36
ATOM   1869   CB    ASN   248     32.147   40.219    6.401   1.00   28.42
ATOM   1870   CG    ASN   248     32.031   41.471    7.253   1.00   29.34
ATOM   1871   OD1   ASN   248     30.975   41.774    7.816   1.00   29.82
ATOM   1872   ND2   ASN   248     33.141   42.201    7.374   1.00   29.54
ATOM   1873   C     ASN   248     29.983   40.798    5.257   1.00   27.10
ATOM   1874   O     ASN   248     30.531   41.618    4.503   1.00   26.98
ATOM   1875   N     THR   249     28.679   40.823    5.544   1.00   26.01
ATOM   1876   CA    THR   249     27.778   41.809    4.937   1.00   23.85
ATOM   1877   CB    THR   249     26.325   41.634    5.424   1.00   23.81
```

Figure 4   Sheet 34 of 62

```
ATOM   1878  OG1  THR   249     26.228  42.100   6.775  1.00  25.10
ATOM   1879  CG2  THR   249     25.899  40.156   5.380  1.00  22.15
ATOM   1880  C    THR   249     28.208  43.226   5.270  1.00  24.20
ATOM   1881  O    THR   249     28.023  44.143   4.467  1.00  23.38
ATOM   1882  N    GLU   250     28.777  43.406   6.462  1.00  24.31
ATOM   1883  CA   GLU   250     29.219  44.733   6.891  1.00  23.61
ATOM   1884  CB   GLU   250     30.446  45.145   6.060  1.00  23.87
ATOM   1885  CG   GLU   250     31.242  46.362   6.571  1.00  25.94
ATOM   1886  CD   GLU   250     32.237  46.041   7.700  1.00  25.83
ATOM   1887  OE1  GLU   250     32.728  44.893   7.813  1.00  25.67
ATOM   1888  OE2  GLU   250     32.552  46.960   8.473  1.00  26.46
ATOM   1889  C    GLU   250     28.003  45.624   6.589  1.00  23.30
ATOM   1890  O    GLU   250     28.110  46.648   5.896  1.00  23.33
ATOM   1891  N    TRP   251     26.841  45.208   7.096  1.00  22.28
ATOM   1892  CA   TRP   251     25.609  45.940   6.840  1.00  22.36
ATOM   1893  CB   TRP   251     24.376  45.077   7.133  1.00  20.65
ATOM   1894  CG   TRP   251     24.133  44.726   8.543  1.00  18.29
ATOM   1895  CD2  TRP   251     23.308  43.648   9.016  1.00  16.51
ATOM   1896  CE2  TRP   251     23.279  43.725  10.424  1.00  15.08
ATOM   1897  CE3  TRP   251     22.589  42.635   8.384  1.00  16.17
ATOM   1898  CD1  TRP   251     24.565  45.395   9.652  1.00  17.71
ATOM   1899  NE1  TRP   251     24.051  44.795  10.795  1.00  17.10
ATOM   1900  CZ2  TRP   251     22.567  42.830  11.201  1.00  14.23
ATOM   1901  CZ3  TRP   251     21.872  41.737   9.171  1.00  15.72
ATOM   1902  CH2  TRP   251     21.869  41.842  10.559  1.00  14.23
ATOM   1903  C    TRP   251     25.445  47.283   7.523  1.00  23.49
ATOM   1904  O    TRP   251     24.541  48.044   7.167  1.00  23.95
ATOM   1905  N    GLY   252     26.302  47.579   8.500  1.00  24.44
ATOM   1906  CA   GLY   252     26.214  48.857   9.179  1.00  25.17
ATOM   1907  C    GLY   252     26.195  49.979   8.152  1.00  26.19
ATOM   1908  O    GLY   252     25.715  51.086   8.429  1.00  26.19
ATOM   1909  N    ALA   253     26.714  49.675   6.960  1.00  26.83
ATOM   1910  CA   ALA   253     26.791  50.622   5.851  1.00  27.86
ATOM   1911  CB   ALA   253     27.822  50.148   4.851  1.00  27.90
ATOM   1912  C    ALA   253     25.448  50.834   5.144  1.00  28.52
ATOM   1913  O    ALA   253     25.249  51.834   4.448  1.00  27.73
ATOM   1914  N    PHE   254     24.536  49.884   5.314  1.00  30.23
ATOM   1915  CA   PHE   254     23.224  49.974   4.696  1.00  31.42
ATOM   1916  CB   PHE   254     22.289  48.947   5.314  1.00  31.71
ATOM   1917  CG   PHE   254     20.899  48.995   4.768  1.00  31.90
ATOM   1918  CD1  PHE   254     20.655  48.736   3.429  1.00  31.47
ATOM   1919  CD2  PHE   254     19.824  49.273   5.600  1.00  32.95
ATOM   1920  CE1  PHE   254     19.367  48.746   2.927  1.00  31.38
ATOM   1921  CE2  PHE   254     18.518  49.285   5.096  1.00  32.69
ATOM   1922  CZ   PHE   254     18.295  49.021   3.763  1.00  31.47
ATOM   1923  C    PHE   254     22.664  51.367   4.928  1.00  32.56
ATOM   1924  O    PHE   254     22.638  51.839   6.064  1.00  33.19
ATOM   1925  N    GLY   255     22.227  52.017   3.849  1.00  33.62
ATOM   1926  CA   GLY   255     21.674  53.354   3.947  1.00  34.98
ATOM   1927  C    GLY   255     22.673  54.429   3.565  1.00  36.85
ATOM   1928  O    GLY   255     22.317  55.604   3.424  1.00  36.70
ATOM   1929  N    ASP   256     23.932  54.038   3.395  1.00  38.95
ATOM   1930  CA   ASP   256     24.966  55.000   3.038  1.00  41.47
ATOM   1931  CB   ASP   256     26.349  54.347   3.088  1.00  41.77
ATOM   1932  CG   ASP   256     26.880  54.224   4.502  1.00  42.36
ATOM   1933  OD1  ASP   256     26.573  55.120   5.322  1.00  43.08
ATOM   1934  OD2  ASP   256     27.617  53.251   4.791  1.00  42.28
```

Figure 4   Sheet 35 of 62

```
ATOM    1935  C    ASP   256      24.744  55.636   1.666  1.00 43.10
ATOM    1936  O    ASP   256      25.489  56.533   1.261  1.00 44.08
ATOM    1937  N    SER   257      23.729  55.171   0.946  1.00 44.19
ATOM    1938  CA   SER   257      23.427  55.738  -0.363  1.00 45.32
ATOM    1939  CB   SER   257      23.714  54.713  -1.467  1.00 45.78
ATOM    1940  OG   SER   257      22.845  53.601  -1.375  1.00 46.48
ATOM    1941  C    SER   257      21.967  56.204  -0.423  1.00 45.41
ATOM    1942  O    SER   257      21.378  56.316  -1.501  1.00 46.14
ATOM    1943  N    GLY   258      21.393  56.466   0.751  1.00 45.52
ATOM    1944  CA   GLY   258      20.018  56.933   0.835  1.00 45.22
ATOM    1945  C    GLY   258      18.922  55.896   1.042  1.00 45.11
ATOM    1946  O    GLY   258      17.745  56.253   1.068  1.00 45.45
ATOM    1947  N    GLU   259      19.284  54.627   1.205  1.00 44.67
ATOM    1948  CA   GLU   259      18.288  53.572   1.380  1.00 44.04
ATOM    1949  CB   GLU   259      18.954  52.187   1.415  1.00 44.23
ATOM    1950  CG   GLU   259      19.952  51.916   0.295  1.00 44.88
ATOM    1951  CD   GLU   259      21.318  52.552   0.548  1.00 45.53
ATOM    1952  OE1  GLU   259      21.381  53.785   0.753  1.00 44.98
ATOM    1953  OE2  GLU   259      22.335  51.817   0.537  1.00 45.95
ATOM    1954  C    GLU   259      17.462  53.749   2.647  1.00 43.91
ATOM    1955  O    GLU   259      16.461  53.061   2.836  1.00 43.49
ATOM    1956  N    LEU   260      17.875  54.661   3.520  1.00 43.87
ATOM    1957  CA   LEU   260      17.143  54.865   4.765  1.00 44.40
ATOM    1958  CB   LEU   260      18.023  54.513   5.967  1.00 44.36
ATOM    1959  CG   LEU   260      18.398  53.041   6.153  1.00 44.87
ATOM    1960  CD1  LEU   260      19.315  52.879   7.369  1.00 44.30
ATOM    1961  CD2  LEU   260      17.127  52.216   6.307  1.00 44.88
ATOM    1962  C    LEU   260      16.632  56.282   4.932  1.00 44.59
ATOM    1963  O    LEU   260      15.744  56.534   5.749  1.00 44.72
ATOM    1964  N    ASP   261      17.200  57.202   4.161  1.00 44.48
ATOM    1965  CA   ASP   261      16.821  58.608   4.234  1.00 44.18
ATOM    1966  CB   ASP   261      16.813  59.224   2.841  1.00 44.99
ATOM    1967  CG   ASP   261      18.192  59.310   2.247  1.00 46.23
ATOM    1968  OD1  ASP   261      19.165  58.994   2.980  1.00 46.42
ATOM    1969  OD2  ASP   261      18.296  59.697   1.055  1.00 46.79
ATOM    1970  C    ASP   261      15.482  58.885   4.892  1.00 43.00
ATOM    1971  O    ASP   261      15.415  59.592   5.898  1.00 42.63
ATOM    1972  N    GLU   262      14.424  58.317   4.320  1.00 41.88
ATOM    1973  CA   GLU   262      13.070  58.525   4.810  1.00 41.00
ATOM    1974  CB   GLU   262      12.088  57.744   3.940  1.00 41.65
ATOM    1975  CG   GLU   262      12.249  56.254   3.999  1.00 43.54
ATOM    1976  CD   GLU   262      11.359  55.562   2.996  1.00 45.44
ATOM    1977  OE1  GLU   262      11.715  55.561   1.800  1.00 47.21
ATOM    1978  OE2  GLU   262      10.296  55.031   3.391  1.00 47.29
ATOM    1979  C    GLU   262      12.830  58.211   6.286  1.00 39.99
ATOM    1980  O    GLU   262      11.997  58.852   6.918  1.00 40.22
ATOM    1981  N    PHE   263      13.545  57.238   6.845  1.00 38.83
ATOM    1982  CA   PHE   263      13.360  56.908   8.258  1.00 37.00
ATOM    1983  CB   PHE   263      13.684  55.430   8.512  1.00 34.37
ATOM    1984  CG   PHE   263      12.828  54.476   7.717  1.00 32.41
ATOM    1985  CD1  PHE   263      13.366  53.753   6.660  1.00 30.67
ATOM    1986  CD2  PHE   263      11.474  54.317   8.012  1.00 30.95
ATOM    1987  CE1  PHE   263      12.567  52.886   5.909  1.00 29.82
ATOM    1988  CE2  PHE   263      10.667  53.450   7.261  1.00 28.87
ATOM    1989  CZ   PHE   263      11.214  52.737   6.213  1.00 29.09
ATOM    1990  C    PHE   263      14.197  57.797   9.190  1.00 36.78
ATOM    1991  O    PHE   263      13.809  58.041  10.327  1.00 37.58
```

Figure 4   Sheet 36 of 62

ATOM	1992	N	LEU	264	15.328	58.301	8.712	1.00	36.72
ATOM	1993	CA	LEU	264	16.193	59.142	9.542	1.00	37.11
ATOM	1994	CB	LEU	264	17.389	59.638	8.725	1.00	36.98
ATOM	1995	CG	LEU	264	18.131	58.621	7.852	1.00	36.59
ATOM	1996	CD1	LEU	264	19.233	59.346	7.077	1.00	35.39
ATOM	1997	CD2	LEU	264	18.701	57.503	8.717	1.00	35.46
ATOM	1998	C	LEU	264	15.482	60.350	10.158	1.00	37.28
ATOM	1999	O	LEU	264	14.879	61.148	9.451	1.00	38.03
ATOM	2000	N	LEU	265	15.574	60.480	11.479	1.00	37.63
ATOM	2001	CA	LEU	265	14.965	61.585	12.215	1.00	37.33
ATOM	2002	CB	LEU	265	14.380	61.070	13.527	1.00	36.25
ATOM	2003	CG	LEU	265	13.529	59.807	13.417	1.00	35.76
ATOM	2004	CD1	LEU	265	13.157	59.295	14.808	1.00	35.17
ATOM	2005	CD2	LEU	265	12.292	60.120	12.598	1.00	35.59
ATOM	2006	C	LEU	265	16.054	62.613	12.521	1.00	38.22
ATOM	2007	O	LEU	265	17.239	62.285	12.486	1.00	38.34
ATOM	2008	N	GLU	266	15.653	63.844	12.832	1.00	39.22
ATOM	2009	CA	GLU	266	16.599	64.922	13.137	1.00	40.56
ATOM	2010	CB	GLU	266	15.874	66.101	13.813	1.00	41.82
ATOM	2011	CG	GLU	266	15.277	65.777	15.196	1.00	44.28
ATOM	2012	CD	GLU	266	14.612	66.974	15.886	1.00	44.95
ATOM	2013	OE1	GLU	266	13.543	67.432	15.410	1.00	45.08
ATOM	2014	OE2	GLU	266	15.163	67.452	16.910	1.00	45.53
ATOM	2015	C	GLU	266	17.733	64.435	14.036	1.00	40.54
ATOM	2016	O	GLU	266	18.910	64.657	13.750	1.00	40.69
ATOM	2017	N	TYR	267	17.366	63.760	15.121	1.00	40.61
ATOM	2018	CA	TYR	267	18.342	63.234	16.062	1.00	40.30
ATOM	2019	CB	TYR	267	17.639	62.364	17.110	1.00	39.44
ATOM	2020	CG	TYR	267	16.216	62.784	17.423	1.00	38.98
ATOM	2021	CD1	TYR	267	15.134	61.967	17.066	1.00	38.66
ATOM	2022	CE1	TYR	267	13.813	62.342	17.349	1.00	38.28
ATOM	2023	CD2	TYR	267	15.943	63.995	18.075	1.00	38.72
ATOM	2024	CE2	TYR	267	14.619	64.381	18.364	1.00	38.45
ATOM	2025	CZ	TYR	267	13.564	63.548	17.996	1.00	38.30
ATOM	2026	OH	TYR	267	12.267	63.923	18.251	1.00	37.22
ATOM	2027	C	TYR	267	19.381	62.403	15.296	1.00	40.27
ATOM	2028	O	TYR	267	20.580	62.469	15.579	1.00	40.14
ATOM	2029	N	ASP	268	18.909	61.626	14.324	1.00	40.61
ATOM	2030	CA	ASP	268	19.781	60.790	13.511	1.00	40.87
ATOM	2031	CB	ASP	268	18.946	59.920	12.566	1.00	39.36
ATOM	2032	CG	ASP	268	18.183	58.843	13.301	1.00	38.52
ATOM	2033	OD1	ASP	268	18.819	58.118	14.082	1.00	39.79
ATOM	2034	OD2	ASP	268	16.961	58.711	13.110	1.00	36.13
ATOM	2035	C	ASP	268	20.764	61.643	12.712	1.00	41.97
ATOM	2036	O	ASP	268	21.956	61.339	12.667	1.00	42.91
ATOM	2037	N	ARG	269	20.266	62.710	12.090	1.00	42.73
ATOM	2038	CA	ARG	269	21.113	63.606	11.310	1.00	43.23
ATOM	2039	CB	ARG	269	20.302	64.793	10.786	1.00	45.34
ATOM	2040	CG	ARG	269	18.923	64.464	10.223	1.00	47.46
ATOM	2041	CD	ARG	269	19.000	63.819	8.864	1.00	49.22
ATOM	2042	NE	ARG	269	17.667	63.552	8.337	1.00	52.67
ATOM	2043	CZ	ARG	269	17.426	62.969	7.165	1.00	54.63
ATOM	2044	NH1	ARG	269	18.436	62.591	6.386	1.00	55.41
ATOM	2045	NH2	ARG	269	16.173	62.747	6.775	1.00	55.38
ATOM	2046	C	ARG	269	22.204	64.150	12.231	1.00	42.99
ATOM	2047	O	ARG	269	23.400	63.999	11.977	1.00	43.63
ATOM	2048	N	LEU	270	21.777	64.796	13.305	1.00	41.99

Figure 4   Sheet 37 of 62

```
ATOM    2049  CA   LEU   270        22.702  65.372  14.261  1.00  41.33
ATOM    2050  CB   LEU   270        21.924  65.812  15.502  1.00  41.15
ATOM    2051  CG   LEU   270        21.004  67.002  15.217  1.00  40.34
ATOM    2052  CD1  LEU   270        19.964  67.182  16.307  1.00  39.94
ATOM    2053  CD2  LEU   270        21.879  68.237  15.084  1.00  40.26
ATOM    2054  C    LEU   270        23.828  64.406  14.635  1.00  41.26
ATOM    2055  O    LEU   270        25.009  64.762  14.553  1.00  41.76
ATOM    2056  N    VAL   271        23.462  63.188  15.030  1.00  40.24
ATOM    2057  CA   VAL   271        24.443  62.177  15.415  1.00  40.08
ATOM    2058  CB   VAL   271        23.776  60.838  15.730  1.00  40.42
ATOM    2059  CG1  VAL   271        24.846  59.800  16.050  1.00  39.86
ATOM    2060  CG2  VAL   271        22.796  61.000  16.891  1.00  40.86
ATOM    2061  C    VAL   271        25.477  61.903  14.329  1.00  40.51
ATOM    2062  O    VAL   271        26.676  61.832  14.595  1.00  40.15
ATOM    2063  N    ASP   272        24.998  61.730  13.103  1.00  40.78
ATOM    2064  CA   ASP   272        25.866  61.447  11.977  1.00  40.36
ATOM    2065  CB   ASP   272        25.038  61.344  10.695  1.00  39.16
ATOM    2066  CG   ASP   272        25.792  60.670   9.553  1.00  38.09
ATOM    2067  OD1  ASP   272        26.821  60.000   9.807  1.00  36.54
ATOM    2068  OD2  ASP   272        25.335  60.798   8.394  1.00  37.12
ATOM    2069  C    ASP   272        26.901  62.544  11.849  1.00  40.88
ATOM    2070  O    ASP   272        28.099  62.297  11.953  1.00  40.75
ATOM    2071  N    GLU   273        26.429  63.763  11.638  1.00  41.96
ATOM    2072  CA   GLU   273        27.321  64.896  11.477  1.00  43.14
ATOM    2073  CB   GLU   273        26.501  66.170  11.470  1.00  44.13
ATOM    2074  CG   GLU   273        25.576  66.214  10.272  1.00  46.73
ATOM    2075  CD   GLU   273        24.629  67.388  10.308  1.00  48.40
ATOM    2076  OE1  GLU   273        25.047  68.455  10.828  1.00  49.15
ATOM    2077  OE2  GLU   273        23.482  67.241   9.811  1.00  48.64
ATOM    2078  C    GLU   273        28.428  64.968  12.517  1.00  43.48
ATOM    2079  O    GLU   273        29.575  65.279  12.187  1.00  43.59
ATOM    2080  N    SER   274        28.095  64.666  13.767  1.00  44.05
ATOM    2081  CA   SER   274        29.089  64.702  14.837  1.00  44.54
ATOM    2082  CB   SER   274        28.421  64.568  16.205  1.00  45.39
ATOM    2083  OG   SER   274        27.496  65.611  16.424  1.00  48.14
ATOM    2084  C    SER   274        30.106  63.582  14.694  1.00  44.23
ATOM    2085  O    SER   274        31.292  63.783  14.931  1.00  44.76
ATOM    2086  N    SER   275        29.632  62.400  14.318  1.00  43.84
ATOM    2087  CA   SER   275        30.489  61.227  14.162  1.00  43.42
ATOM    2088  CB   SER   275        29.754  60.139  13.392  1.00  43.28
ATOM    2089  OG   SER   275        29.758  60.444  12.010  1.00  42.94
ATOM    2090  C    SER   275        31.789  61.535  13.426  1.00  43.34
ATOM    2091  O    SER   275        31.914  62.552  12.738  1.00  43.76
ATOM    2092  N    ALA   276        32.756  60.639  13.570  1.00  42.68
ATOM    2093  CA   ALA   276        34.034  60.805  12.906  1.00  42.98
ATOM    2094  CB   ALA   276        35.108  60.015  13.639  1.00  42.92
ATOM    2095  C    ALA   276        33.930  60.319  11.465  1.00  43.23
ATOM    2096  O    ALA   276        34.936  60.277  10.751  1.00  44.60
ATOM    2097  N    ASN   277        32.722  59.949  11.039  1.00  42.10
ATOM    2098  CA   ASN   277        32.517  59.447   9.691  1.00  40.87
ATOM    2099  CB   ASN   277        32.615  57.927   9.685  1.00  41.63
ATOM    2100  CG   ASN   277        31.654  57.283  10.659  1.00  42.64
ATOM    2101  OD1  ASN   277        30.670  57.898  11.067  1.00  43.50
ATOM    2102  ND2  ASN   277        31.925  56.033  11.029  1.00  42.98
ATOM    2103  C    ASN   277        31.178  59.865   9.104  1.00  40.57
ATOM    2104  O    ASN   277        30.430  59.039   8.579  1.00  39.89
ATOM    2105  N    PRO   278        30.868  61.163   9.163  1.00  40.83
```

Figure 4   Sheet 38 of 62

```
ATOM   2106  CD  PRO  278    31.783  62.282   9.451  1.00  40.90
ATOM   2107  CA  PRO  278    29.600  61.657   8.623  1.00  40.71
ATOM   2108  CB  PRO  278    29.807  63.175   8.579  1.00  40.88
ATOM   2109  CG  PRO  278    31.303  63.326   8.474  1.00  41.27
ATOM   2110  C   PRO  278    29.239  61.074   7.258  1.00  40.60
ATOM   2111  O   PRO  278    29.949  61.284   6.270  1.00  40.71
ATOM   2112  N   GLY  279    28.131  60.338   7.216  1.00  40.34
ATOM   2113  CA  GLY  279    27.676  59.747   5.971  1.00  39.10
ATOM   2114  C   GLY  279    27.904  58.252   5.828  1.00  38.94
ATOM   2115  O   GLY  279    27.315  57.635   4.952  1.00  39.74
ATOM   2116  N   GLN  280    28.735  57.660   6.683  1.00  38.66
ATOM   2117  CA  GLN  280    29.049  56.230   6.605  1.00  37.75
ATOM   2118  CB  GLN  280    30.563  56.043   6.513  1.00  37.97
ATOM   2119  CG  GLN  280    31.243  56.954   5.509  1.00  39.85
ATOM   2120  CD  GLN  280    32.743  57.046   5.730  1.00  40.76
ATOM   2121  OE1 GLN  280    33.465  56.058   5.587  1.00  41.39
ATOM   2122  NE2 GLN  280    33.220  58.240   6.083  1.00  41.57
ATOM   2123  C   GLN  280    28.553  55.455   7.817  1.00  36.99
ATOM   2124  O   GLN  280    28.645  55.939   8.941  1.00  37.89
ATOM   2125  N   GLN  281    28.054  54.242   7.592  1.00  35.75
ATOM   2126  CA  GLN  281    27.572  53.401   8.681  1.00  34.04
ATOM   2127  CB  GLN  281    28.590  53.404   9.829  1.00  33.35
ATOM   2128  CG  GLN  281    29.971  52.951   9.447  1.00  33.09
ATOM   2129  CD  GLN  281    29.967  51.576   8.800  1.00  34.44
ATOM   2130  OE1 GLN  281    29.917  51.451   7.572  1.00  33.95
ATOM   2131  NE2 GLN  281    30.000  50.529   9.630  1.00  34.63
ATOM   2132  C   GLN  281    26.210  53.831   9.237  1.00  33.42
ATOM   2133  O   GLN  281    25.895  53.530  10.390  1.00  34.87
ATOM   2134  N   LEU  282    25.395  54.511   8.436  1.00  31.53
ATOM   2135  CA  LEU  282    24.098  54.992   8.913  1.00  29.87
ATOM   2136  CB  LEU  282    23.345  55.685   7.777  1.00  30.15
ATOM   2137  CG  LEU  282    24.030  56.871   7.085  1.00  30.41
ATOM   2138  CD1 LEU  282    22.963  57.741   6.435  1.00  29.82
ATOM   2139  CD2 LEU  282    24.815  57.699   8.097  1.00  30.66
ATOM   2140  C   LEU  282    23.191  53.949   9.578  1.00  28.70
ATOM   2141  O   LEU  282    22.716  54.153  10.698  1.00  28.78
ATOM   2142  N   TYR  283    22.935  52.841   8.894  1.00  27.35
ATOM   2143  CA  TYR  283    22.095  51.793   9.461  1.00  26.53
ATOM   2144  CB  TYR  283    22.233  50.511   8.633  1.00  24.41
ATOM   2145  CG  TYR  283    21.420  49.338   9.143  1.00  22.90
ATOM   2146  CD1 TYR  283    20.021  49.413   9.210  1.00  21.94
ATOM   2147  CE1 TYR  283    19.257  48.318   9.609  1.00  20.96
ATOM   2148  CD2 TYR  283    22.038  48.129   9.503  1.00  21.53
ATOM   2149  CE2 TYR  283    21.279  47.030   9.907  1.00  20.87
ATOM   2150  CZ  TYR  283    19.886  47.140   9.950  1.00  21.33
ATOM   2151  OH  TYR  283    19.105  46.068  10.310  1.00  23.85
ATOM   2152  C   TYR  283    22.567  51.532  10.891  1.00  27.12
ATOM   2153  O   TYR  283    21.783  51.521  11.841  1.00  28.95
ATOM   2154  N   GLU  284    23.869  51.352  11.035  1.00  26.60
ATOM   2155  CA  GLU  284    24.486  51.072  12.317  1.00  26.43
ATOM   2156  CB  GLU  284    25.982  50.905  12.108  1.00  27.03
ATOM   2157  CG  GLU  284    26.763  50.680  13.375  1.00  27.21
ATOM   2158  CD  GLU  284    28.224  50.492  13.082  1.00  27.57
ATOM   2159  OE1 GLU  284    28.897  51.506  12.734  1.00  27.02
ATOM   2160  OE2 GLU  284    28.670  49.319  13.185  1.00  26.30
ATOM   2161  C   GLU  284    24.249  52.133  13.381  1.00  26.81
ATOM   2162  O   GLU  284    24.197  51.826  14.582  1.00  26.06
```

Figure 4   Sheet 39 of 62

```
ATOM  2163  N    LYS  285    24.134  53.384  12.940  1.00  27.07
ATOM  2164  CA   LYS  285    23.926  54.502  13.860  1.00  27.39
ATOM  2165  CB   LYS  285    24.339  55.825  13.186  1.00  25.99
ATOM  2166  CG   LYS  285    25.840  56.012  13.132  1.00  24.13
ATOM  2167  CD   LYS  285    26.235  57.110  12.179  1.00  23.29
ATOM  2168  CE   LYS  285    27.755  57.193  12.052  1.00  22.03
ATOM  2169  NZ   LYS  285    28.142  58.198  11.027  1.00  21.72
ATOM  2170  C    LYS  285    22.488  54.595  14.368  1.00  28.05
ATOM  2171  O    LYS  285    22.086  55.615  14.941  1.00  28.61
ATOM  2172  N    LEU  286    21.717  53.535  14.144  1.00  27.60
ATOM  2173  CA   LEU  286    20.335  53.488  14.599  1.00  27.30
ATOM  2174  CB   LEU  286    19.399  53.157  13.435  1.00  28.57
ATOM  2175  CG   LEU  286    19.375  54.167  12.279  1.00  30.25
ATOM  2176  CD1  LEU  286    18.480  53.647  11.139  1.00  29.98
ATOM  2177  CD2  LEU  286    18.863  55.507  12.780  1.00  29.35
ATOM  2178  C    LEU  286    20.260  52.381  15.632  1.00  27.01
ATOM  2179  O    LEU  286    19.296  52.294  16.399  1.00  27.55
ATOM  2180  N    ILE  287    21.306  51.554  15.645  1.00  26.00
ATOM  2181  CA   ILE  287    21.415  50.399  16.532  1.00  24.38
ATOM  2182  CB   ILE  287    21.551  49.141  15.715  1.00  23.92
ATOM  2183  CG2  ILE  287    21.470  47.919  16.628  1.00  22.70
ATOM  2184  CG1  ILE  287    20.510  49.158  14.597  1.00  22.87
ATOM  2185  CD1  ILE  287    20.676  48.042  13.607  1.00  22.79
ATOM  2186  C    ILE  287    22.639  50.444  17.433  1.00  24.65
ATOM  2187  O    ILE  287    22.550  50.255  18.644  1.00  23.54
ATOM  2188  N    GLY  288    23.791  50.668  16.810  1.00  25.94
ATOM  2189  CA   GLY  288    25.060  50.714  17.519  1.00  26.86
ATOM  2190  C    GLY  288    25.081  51.266  18.927  1.00  27.76
ATOM  2191  O    GLY  288    24.697  52.412  19.164  1.00  28.19
ATOM  2192  N    GLY  289    25.554  50.445  19.860  1.00  28.95
ATOM  2193  CA   GLY  289    25.656  50.856  21.249  1.00  30.64
ATOM  2194  C    GLY  289    26.632  52.007  21.407  1.00  31.92
ATOM  2195  O    GLY  289    26.930  52.442  22.509  1.00  32.56
ATOM  2196  N    LYS  290    27.133  52.504  20.291  1.00  32.83
ATOM  2197  CA   LYS  290    28.067  53.607  20.296  1.00  33.99
ATOM  2198  CB   LYS  290    29.104  53.373  19.191  1.00  35.04
ATOM  2199  CG   LYS  290    29.858  54.598  18.665  1.00  36.71
ATOM  2200  CD   LYS  290    31.032  54.996  19.551  1.00  38.80
ATOM  2201  CE   LYS  290    31.936  56.011  18.839  1.00  39.77
ATOM  2202  NZ   LYS  290    32.864  56.707  19.787  1.00  41.04
ATOM  2203  C    LYS  290    27.278  54.880  20.035  1.00  34.58
ATOM  2204  O    LYS  290    27.810  55.984  20.138  1.00  35.79
ATOM  2205  N    TYR  291    26.001  54.734  19.708  1.00  33.80
ATOM  2206  CA   TYR  291    25.196  55.907  19.406  1.00  33.61
ATOM  2207  CB   TYR  291    25.010  56.046  17.892  1.00  33.22
ATOM  2208  CG   TYR  291    26.256  55.752  17.084  1.00  33.77
ATOM  2209  CD1  TYR  291    26.659  54.435  16.838  1.00  34.23
ATOM  2210  CE1  TYR  291    27.789  54.155  16.065  1.00  34.17
ATOM  2211  CD2  TYR  291    27.021  56.783  16.542  1.00  33.61
ATOM  2212  CE2  TYR  291    28.150  56.515  15.773  1.00  33.54
ATOM  2213  CZ   TYR  291    28.528  55.200  15.532  1.00  33.76
ATOM  2214  OH   TYR  291    29.620  54.928  14.729  1.00  34.36
ATOM  2215  C    TYR  291    23.836  55.874  20.070  1.00  33.11
ATOM  2216  O    TYR  291    23.069  56.828  19.975  1.00  32.86
ATOM  2217  N    MSE  292    23.521  54.778  20.737  1.00  33.27
ATOM  2218  CA   MSE  292    22.230  54.699  21.389  1.00  33.18
ATOM  2219  CB   MSE  292    22.066  53.349  22.062  1.00  33.77
```

Figure 4   Sheet 40 of 62

```
ATOM    2220  CG   MSE   292      20.639  52.975  22.314  1.00  35.15
ATOM    2221  SE   MSE   292      20.564  51.230  22.803  1.00  41.54
ATOM    2222  CE   MSE   292      20.269  50.385  21.171  1.00  35.91
ATOM    2223  C    MSE   292      22.148  55.818  22.423  1.00  32.97
ATOM    2224  O    MSE   292      21.227  56.637  22.400  1.00  33.49
ATOM    2225  N    GLY   293      23.131  55.861  23.315  1.00  32.96
ATOM    2226  CA   GLY   293      23.151  56.892  24.334  1.00  32.25
ATOM    2227  C    GLY   293      23.067  58.290  23.750  1.00  32.18
ATOM    2228  O    GLY   293      22.307  59.126  24.241  1.00  33.24
ATOM    2229  N    GLU   294      23.835  58.560  22.702  1.00  31.47
ATOM    2230  CA   GLU   294      23.809  59.883  22.096  1.00  31.38
ATOM    2231  CB   GLU   294      24.875  59.971  21.008  1.00  33.29
ATOM    2232  CG   GLU   294      24.986  61.321  20.304  1.00  34.67
ATOM    2233  CD   GLU   294      25.227  62.474  21.257  1.00  35.80
ATOM    2234  OE1  GLU   294      25.708  62.244  22.389  1.00  36.49
ATOM    2235  OE2  GLU   294      24.946  63.623  20.858  1.00  37.16
ATOM    2236  C    GLU   294      22.428  60.192  21.521  1.00  30.62
ATOM    2237  O    GLU   294      21.919  61.305  21.664  1.00  30.94
ATOM    2238  N    LEU   295      21.818  59.204  20.878  1.00  29.56
ATOM    2239  CA   LEU   295      20.495  59.392  20.303  1.00  29.24
ATOM    2240  CB   LEU   295      20.030  58.112  19.589  1.00  27.27
ATOM    2241  CG   LEU   295      20.389  58.007  18.099  1.00  25.46
ATOM    2242  CD1  LEU   295      19.979  56.668  17.522  1.00  21.87
ATOM    2243  CD2  LEU   295      19.677  59.136  17.352  1.00  25.71
ATOM    2244  C    LEU   295      19.497  59.787  21.388  1.00  29.98
ATOM    2245  O    LEU   295      18.587  60.573  21.156  1.00  30.19
ATOM    2246  N    VAL   296      19.665  59.250  22.585  1.00  31.23
ATOM    2247  CA   VAL   296      18.745  59.590  23.657  1.00  32.87
ATOM    2248  CB   VAL   296      18.890  58.623  24.831  1.00  32.48
ATOM    2249  CG1  VAL   296      17.827  58.899  25.868  1.00  32.99
ATOM    2250  CG2  VAL   296      18.762  57.198  24.323  1.00  33.56
ATOM    2251  C    VAL   296      19.020  61.025  24.122  1.00  33.74
ATOM    2252  O    VAL   296      18.086  61.778  24.431  1.00  33.68
ATOM    2253  N    ARG   297      20.296  61.409  24.145  1.00  34.02
ATOM    2254  CA   ARG   297      20.659  62.757  24.563  1.00  35.34
ATOM    2255  CB   ARG   297      22.147  63.008  24.342  1.00  34.89
ATOM    2256  CG   ARG   297      22.940  63.279  25.609  1.00  35.27
ATOM    2257  CD   ARG   297      23.791  64.525  25.454  1.00  35.98
ATOM    2258  NE   ARG   297      24.226  64.700  24.074  1.00  37.11
ATOM    2259  CZ   ARG   297      24.476  65.878  23.513  1.00  37.43
ATOM    2260  NH1  ARG   297      24.348  66.994  24.226  1.00  38.45
ATOM    2261  NH2  ARG   297      24.809  65.944  22.229  1.00  36.61
ATOM    2262  C    ARG   297      19.870  63.766  23.747  1.00  36.07
ATOM    2263  O    ARG   297      19.103  64.574  24.285  1.00  36.76
ATOM    2264  N    LEU   298      20.063  63.699  22.437  1.00  36.93
ATOM    2265  CA   LEU   298      19.407  64.596  21.500  1.00  37.55
ATOM    2266  CB   LEU   298      19.768  64.178  20.077  1.00  37.28
ATOM    2267  CG   LEU   298      21.272  64.065  19.816  1.00  36.13
ATOM    2268  CD1  LEU   298      21.478  63.784  18.341  1.00  36.85
ATOM    2269  CD2  LEU   298      21.991  65.356  20.218  1.00  35.02
ATOM    2270  C    LEU   298      17.892  64.633  21.670  1.00  38.53
ATOM    2271  O    LEU   298      17.276  65.708  21.618  1.00  38.44
ATOM    2272  N    VAL   299      17.289  63.462  21.866  1.00  39.23
ATOM    2273  CA   VAL   299      15.839  63.389  22.054  1.00  40.08
ATOM    2274  CB   VAL   299      15.349  61.932  22.110  1.00  39.44
ATOM    2275  CG1  VAL   299      13.844  61.892  22.385  1.00  37.91
ATOM    2276  CG2  VAL   299      15.676  61.240  20.802  1.00  38.72
```

Figure 4   Sheet 41 of 62

```
ATOM    2277  C   VAL   299      15.435  64.087  23.350  1.00  40.94
ATOM    2278  O   VAL   299      14.321  64.612  23.461  1.00  41.66
ATOM    2279  N   LEU   300      16.337  64.091  24.328  1.00  41.41
ATOM    2280  CA  LEU   300      16.043  64.737  25.600  1.00  42.31
ATOM    2281  CB  LEU   300      16.973  64.224  26.713  1.00  41.48
ATOM    2282  CG  LEU   300      16.943  62.766  27.206  1.00  40.38
ATOM    2283  CD1 LEU   300      17.677  62.711  28.545  1.00  40.14
ATOM    2284  CD2 LEU   300      15.517  62.251  27.380  1.00  38.74
ATOM    2285  C   LEU   300      16.204  66.251  25.444  1.00  43.44
ATOM    2286  O   LEU   300      15.304  67.020  25.806  1.00  43.84
ATOM    2287  N   LEU   301      17.346  66.675  24.898  1.00  43.90
ATOM    2288  CA  LEU   301      17.603  68.100  24.707  1.00  43.85
ATOM    2289  CB  LEU   301      18.895  68.335  23.919  1.00  43.20
ATOM    2290  CG  LEU   301      20.211  67.969  24.613  1.00  43.48
ATOM    2291  CD1 LEU   301      21.385  68.372  23.730  1.00  43.37
ATOM    2292  CD2 LEU   301      20.307  68.675  25.955  1.00  43.71
ATOM    2293  C   LEU   301      16.444  68.738  23.969  1.00  44.11
ATOM    2294  O   LEU   301      16.068  69.875  24.254  1.00  44.38
ATOM    2295  N   ARG   302      15.863  68.007  23.025  1.00  44.45
ATOM    2296  CA  ARG   302      14.753  68.571  22.280  1.00  45.04
ATOM    2297  CB  ARG   302      14.296  67.660  21.148  1.00  45.49
ATOM    2298  CG  ARG   302      13.082  68.256  20.468  1.00  45.91
ATOM    2299  CD  ARG   302      12.391  67.327  19.514  1.00  46.45
ATOM    2300  NE  ARG   302      11.194  67.985  19.007  1.00  47.37
ATOM    2301  CZ  ARG   302      10.423  67.503  18.043  1.00  48.12
ATOM    2302  NH1 ARG   302      10.719  66.344  17.466  1.00  48.80
ATOM    2303  NH2 ARG   302       9.357  68.190  17.657  1.00  47.77
ATOM    2304  C   ARG   302      13.577  68.807  23.196  1.00  45.13
ATOM    2305  O   ARG   302      12.982  69.885  23.198  1.00  45.57
ATOM    2306  N   LEU   303      13.228  67.787  23.966  1.00  45.14
ATOM    2307  CA  LEU   303      12.113  67.918  24.883  1.00  45.18
ATOM    2308  CB  LEU   303      11.952  66.624  25.695  1.00  44.02
ATOM    2309  CG  LEU   303      11.495  65.427  24.846  1.00  42.43
ATOM    2310  CD1 LEU   303      11.365  64.162  25.690  1.00  41.06
ATOM    2311  CD2 LEU   303      10.154  65.784  24.207  1.00  41.96
ATOM    2312  C   LEU   303      12.359  69.133  25.783  1.00  45.83
ATOM    2313  O   LEU   303      11.444  69.919  26.044  1.00  45.85
ATOM    2314  N   VAL   304      13.599  69.302  26.232  1.00  46.44
ATOM    2315  CA  VAL   304      13.943  70.440  27.085  1.00  47.76
ATOM    2316  CB  VAL   304      15.443  70.426  27.496  1.00  47.79
ATOM    2317  CG1 VAL   304      15.866  71.815  27.996  1.00  46.89
ATOM    2318  CG2 VAL   304      15.678  69.386  28.581  1.00  47.81
ATOM    2319  C   VAL   304      13.666  71.764  26.371  1.00  48.44
ATOM    2320  O   VAL   304      12.899  72.596  26.861  1.00  48.95
ATOM    2321  N   ASP   305      14.297  71.946  25.212  1.00  48.52
ATOM    2322  CA  ASP   305      14.143  73.165  24.432  1.00  48.31
ATOM    2323  CB  ASP   305      14.968  73.067  23.143  1.00  49.45
ATOM    2324  CG  ASP   305      16.441  72.715  23.412  1.00  51.00
ATOM    2325  OD1 ASP   305      17.056  73.323  24.317  1.00  50.99
ATOM    2326  OD2 ASP   305      16.994  71.834  22.715  1.00  51.84
ATOM    2327  C   ASP   305      12.677  73.460  24.122  1.00  47.77
ATOM    2328  O   ASP   305      12.341  74.541  23.641  1.00  48.22
ATOM    2329  N   GLU   306      11.799  72.505  24.407  1.00  46.84
ATOM    2330  CA  GLU   306      10.378  72.713  24.176  1.00  46.34
ATOM    2331  CB  GLU   306       9.831  71.683  23.184  1.00  46.20
ATOM    2332  CG  GLU   306       9.866  72.216  21.761  1.00  48.15
ATOM    2333  CD  GLU   306       9.571  71.175  20.692  1.00  49.26
```

Figure 4   Sheet 42 of 62

ATOM	2334	OE1	GLU	306	8.514	70.499	20.768	1.00	50.03
ATOM	2335	OE2	GLU	306	10.398	71.049	19.759	1.00	49.62
ATOM	2336	C	GLU	306	9.635	72.661	25.493	1.00	45.99
ATOM	2337	O	GLU	306	8.459	72.331	25.550	1.00	45.90
ATOM	2338	N	ASN	307	10.350	72.997	26.560	1.00	46.00
ATOM	2339	CA	ASN	307	9.787	73.029	27.902	1.00	45.60
ATOM	2340	CB	ASN	307	9.033	74.342	28.094	1.00	46.42
ATOM	2341	CG	ASN	307	9.971	75.531	28.224	1.00	46.98
ATOM	2342	OD1	ASN	307	10.435	75.849	29.321	1.00	47.63
ATOM	2343	ND2	ASN	307	10.273	76.181	27.102	1.00	46.93
ATOM	2344	C	ASN	307	8.886	71.853	28.246	1.00	45.05
ATOM	2345	O	ASN	307	7.812	72.029	28.829	1.00	45.19
ATOM	2346	N	LEU	308	9.336	70.650	27.900	1.00	44.24
ATOM	2347	CA	LEU	308	8.575	69.439	28.180	1.00	43.28
ATOM	2348	CB	LEU	308	8.376	68.637	26.893	1.00	43.27
ATOM	2349	CG	LEU	308	7.070	68.825	26.115	1.00	44.09
ATOM	2350	CD1	LEU	308	6.765	70.294	25.935	1.00	44.22
ATOM	2351	CD2	LEU	308	7.182	68.139	24.760	1.00	43.94
ATOM	2352	C	LEU	308	9.287	68.570	29.205	1.00	42.96
ATOM	2353	O	LEU	308	8.688	67.660	29.775	1.00	42.27
ATOM	2354	N	LEU	309	10.560	68.868	29.448	1.00	43.49
ATOM	2355	CA	LEU	309	11.368	68.077	30.371	1.00	44.85
ATOM	2356	CB	LEU	309	12.030	66.936	29.581	1.00	43.53
ATOM	2357	CG	LEU	309	12.958	65.925	30.254	1.00	42.07
ATOM	2358	CD1	LEU	309	12.235	65.226	31.390	1.00	40.83
ATOM	2359	CD2	LEU	309	13.416	64.913	29.212	1.00	42.11
ATOM	2360	C	LEU	309	12.436	68.900	31.108	1.00	46.21
ATOM	2361	O	LEU	309	13.074	69.777	30.518	1.00	46.04
ATOM	2362	N	PHE	310	12.625	68.601	32.397	1.00	47.92
ATOM	2363	CA	PHE	310	13.608	69.293	33.238	1.00	49.25
ATOM	2364	CB	PHE	310	15.013	69.093	32.666	1.00	48.20
ATOM	2365	CG	PHE	310	15.438	67.650	32.590	1.00	47.06
ATOM	2366	CD1	PHE	310	16.338	67.228	31.615	1.00	46.24
ATOM	2367	CD2	PHE	310	14.947	66.715	33.497	1.00	46.63
ATOM	2368	CE1	PHE	310	16.740	65.903	31.540	1.00	45.74
ATOM	2369	CE2	PHE	310	15.344	65.385	33.433	1.00	46.27
ATOM	2370	CZ	PHE	310	16.243	64.978	32.451	1.00	45.93
ATOM	2371	C	PHE	310	13.292	70.785	33.345	1.00	51.16
ATOM	2372	O	PHE	310	14.185	71.616	33.561	1.00	50.84
ATOM	2373	N	HIS	311	12.009	71.109	33.183	1.00	53.40
ATOM	2374	CA	HIS	311	11.529	72.482	33.262	1.00	55.80
ATOM	2375	CB	HIS	311	11.744	73.012	34.683	1.00	57.57
ATOM	2376	CG	HIS	311	11.212	72.098	35.745	1.00	59.78
ATOM	2377	CD2	HIS	311	11.848	71.363	36.689	1.00	60.29
ATOM	2378	ND1	HIS	311	9.867	71.815	35.879	1.00	60.36
ATOM	2379	CE1	HIS	311	9.699	70.944	36.860	1.00	60.99
ATOM	2380	NE2	HIS	311	10.885	70.654	37.368	1.00	60.85
ATOM	2381	C	HIS	311	12.214	73.384	32.236	1.00	56.24
ATOM	2382	O	HIS	311	12.288	74.608	32.415	1.00	56.87
ATOM	2383	N	GLY	312	12.705	72.772	31.159	1.00	55.96
ATOM	2384	CA	GLY	312	13.366	73.522	30.109	1.00	55.87
ATOM	2385	C	GLY	312	14.820	73.804	30.420	1.00	56.16
ATOM	2386	O	GLY	312	15.563	74.264	29.562	1.00	56.58
ATOM	2387	N	GLU	313	15.235	73.519	31.646	1.00	56.52
ATOM	2388	CA	GLU	313	16.612	73.765	32.048	1.00	57.69
ATOM	2389	CB	GLU	313	16.621	74.379	33.447	1.00	59.84
ATOM	2390	CG	GLU	313	15.849	75.698	33.515	1.00	63.16

Figure 4   Sheet 43 of 62

ATOM	2391	CD	GLU	313	15.388	76.061	34.925	1.00	65.16
ATOM	2392	OE1	GLU	313	14.554	75.315	35.503	1.00	66.01
ATOM	2393	OE2	GLU	313	15.858	77.096	35.455	1.00	66.34
ATOM	2394	C	GLU	313	17.439	72.484	32.011	1.00	57.06
ATOM	2395	O	GLU	313	17.155	71.529	32.728	1.00	57.01
ATOM	2396	N	ALA	314	18.463	72.472	31.169	1.00	56.56
ATOM	2397	CA	ALA	314	19.316	71.305	31.029	1.00	56.76
ATOM	2398	CB	ALA	314	19.454	70.939	29.557	1.00	56.47
ATOM	2399	C	ALA	314	20.699	71.490	31.643	1.00	56.94
ATOM	2400	O	ALA	314	21.310	72.558	31.527	1.00	57.46
ATOM	2401	N	SER	315	21.183	70.422	32.276	1.00	56.73
ATOM	2402	CA	SER	315	22.487	70.383	32.932	1.00	56.15
ATOM	2403	CB	SER	315	22.666	69.029	33.624	1.00	56.44
ATOM	2404	OG	SER	315	23.981	68.868	34.130	1.00	57.39
ATOM	2405	C	SER	315	23.673	70.627	32.003	1.00	56.00
ATOM	2406	O	SER	315	23.595	70.416	30.793	1.00	55.42
ATOM	2407	N	GLU	316	24.776	71.070	32.598	1.00	56.67
ATOM	2408	CA	GLU	316	26.012	71.346	31.875	1.00	57.46
ATOM	2409	CB	GLU	316	27.111	71.754	32.860	1.00	58.71
ATOM	2410	CG	GLU	316	28.458	72.050	32.206	1.00	60.34
ATOM	2411	CD	GLU	316	28.442	73.343	31.406	1.00	61.64
ATOM	2412	OE1	GLU	316	28.288	74.420	32.031	1.00	62.41
ATOM	2413	OE2	GLU	316	28.574	73.280	30.160	1.00	61.76
ATOM	2414	C	GLU	316	26.442	70.078	31.161	1.00	57.35
ATOM	2415	O	GLU	316	26.770	70.088	29.972	1.00	57.68
ATOM	2416	N	GLN	317	26.439	68.988	31.920	1.00	56.84
ATOM	2417	CA	GLN	317	26.817	67.677	31.427	1.00	56.23
ATOM	2418	CB	GLN	317	26.760	66.669	32.580	1.00	55.93
ATOM	2419	CG	GLN	317	27.504	67.113	33.840	1.00	55.46
ATOM	2420	CD	GLN	317	27.063	66.355	35.085	1.00	55.01
ATOM	2421	OE1	GLN	317	27.246	65.140	35.194	1.00	54.83
ATOM	2422	NE2	GLN	317	26.468	67.074	36.029	1.00	54.68
ATOM	2423	C	GLN	317	25.902	67.210	30.290	1.00	56.37
ATOM	2424	O	GLN	317	26.376	66.634	29.312	1.00	56.16
ATOM	2425	N	LEU	318	24.599	67.476	30.412	1.00	56.41
ATOM	2426	CA	LEU	318	23.616	67.043	29.413	1.00	56.48
ATOM	2427	CB	LEU	318	22.190	67.333	29.890	1.00	55.59
ATOM	2428	CG	LEU	318	21.084	66.700	29.034	1.00	54.71
ATOM	2429	CD1	LEU	318	21.090	65.191	29.231	1.00	53.88
ATOM	2430	CD2	LEU	318	19.731	67.268	29.422	1.00	54.28
ATOM	2431	C	LEU	318	23.784	67.621	28.017	1.00	56.99
ATOM	2432	O	LEU	318	23.692	66.893	27.029	1.00	57.21
ATOM	2433	N	ARG	319	24.011	68.924	27.919	1.00	57.16
ATOM	2434	CA	ARG	319	24.177	69.530	26.606	1.00	57.68
ATOM	2435	CB	ARG	319	23.870	71.026	26.690	1.00	59.32
ATOM	2436	CG	ARG	319	22.420	71.284	27.105	1.00	62.20
ATOM	2437	CD	ARG	319	22.125	72.743	27.401	1.00	64.53
ATOM	2438	NE	ARG	319	20.758	72.927	27.892	1.00	66.89
ATOM	2439	CZ	ARG	319	20.297	74.055	28.433	1.00	68.29
ATOM	2440	NH1	ARG	319	21.096	75.112	28.555	1.00	68.30
ATOM	2441	NH2	ARG	319	19.034	74.127	28.851	1.00	68.25
ATOM	2442	C	ARG	319	25.587	69.278	26.081	1.00	57.09
ATOM	2443	O	ARG	319	26.049	69.951	25.160	1.00	57.05
ATOM	2444	N	THR	320	26.246	68.277	26.667	1.00	56.25
ATOM	2445	CA	THR	320	27.612	67.888	26.318	1.00	55.15
ATOM	2446	CB	THR	320	28.478	67.836	27.589	1.00	54.85
ATOM	2447	OG1	THR	320	28.601	69.158	28.133	1.00	54.94

Figure 4   Sheet 44 of 62

ATOM	2448	CG2	THR	320	29.854	67.262	27.287	1.00 54.63
ATOM	2449	C	THR	320	27.689	66.524	25.613	1.00 55.04
ATOM	2450	O	THR	320	27.476	65.480	26.229	1.00 55.13
ATOM	2451	N	ARG	321	28.017	66.536	24.326	1.00 54.38
ATOM	2452	CA	ARG	321	28.106	65.304	23.545	1.00 54.36
ATOM	2453	CB	ARG	321	28.841	65.586	22.236	1.00 56.05
ATOM	2454	CG	ARG	321	28.153	66.651	21.402	1.00 59.03
ATOM	2455	CD	ARG	321	28.943	67.013	20.156	1.00 61.60
ATOM	2456	NE	ARG	321	28.331	68.123	19.426	1.00 63.68
ATOM	2457	CZ	ARG	321	28.909	68.753	18.406	1.00 65.43
ATOM	2458	NH1	ARG	321	30.119	68.381	17.997	1.00 65.83
ATOM	2459	NH2	ARG	321	28.280	69.750	17.792	1.00 65.76
ATOM	2460	C	ARG	321	28.765	64.123	24.262	1.00 52.97
ATOM	2461	O	ARG	321	29.885	64.234	24.758	1.00 53.13
ATOM	2462	N	GLY	322	28.056	62.996	24.316	1.00 51.39
ATOM	2463	CA	GLY	322	28.592	61.802	24.950	1.00 49.22
ATOM	2464	C	GLY	322	28.198	61.609	26.402	1.00 48.17
ATOM	2465	O	GLY	322	28.450	60.550	26.986	1.00 48.17
ATOM	2466	N	ALA	323	27.574	62.627	26.988	1.00 46.66
ATOM	2467	CA	ALA	323	27.150	62.573	28.385	1.00 44.99
ATOM	2468	CB	ALA	323	26.462	63.861	28.761	1.00 45.87
ATOM	2469	C	ALA	323	26.224	61.403	28.676	1.00 43.43
ATOM	2470	O	ALA	323	26.514	60.562	29.530	1.00 43.02
ATOM	2471	N	PHE	324	25.094	61.361	27.981	1.00 41.61
ATOM	2472	CA	PHE	324	24.147	60.282	28.185	1.00 40.44
ATOM	2473	CB	PHE	324	22.797	60.631	27.564	1.00 38.94
ATOM	2474	CG	PHE	324	21.644	59.988	28.262	1.00 38.08
ATOM	2475	CD1	PHE	324	21.047	60.613	29.360	1.00 37.48
ATOM	2476	CD2	PHE	324	21.185	58.733	27.860	1.00 36.96
ATOM	2477	CE1	PHE	324	20.010	59.998	30.050	1.00 37.11
ATOM	2478	CE2	PHE	324	20.146	58.105	28.542	1.00 37.79
ATOM	2479	CZ	PHE	324	19.555	58.739	29.643	1.00 37.73
ATOM	2480	C	PHE	324	24.721	59.033	27.525	1.00 40.11
ATOM	2481	O	PHE	324	24.785	58.937	26.289	1.00 40.76
ATOM	2482	N	GLU	325	25.129	58.072	28.350	1.00 39.06
ATOM	2483	CA	GLU	325	25.740	56.851	27.844	1.00 37.85
ATOM	2484	CB	GLU	325	26.846	56.418	28.781	1.00 38.17
ATOM	2485	CG	GLU	325	27.790	57.528	29.085	1.00 40.68
ATOM	2486	CD	GLU	325	28.922	57.075	29.951	1.00 42.47
ATOM	2487	OE1	GLU	325	28.653	56.608	31.086	1.00 44.06
ATOM	2488	OE2	GLU	325	30.080	57.181	29.490	1.00 44.51
ATOM	2489	C	GLU	325	24.799	55.693	27.641	1.00 36.60
ATOM	2490	O	GLU	325	23.903	55.445	28.447	1.00 37.31
ATOM	2491	N	THR	326	25.019	54.968	26.554	1.00 35.30
ATOM	2492	CA	THR	326	24.193	53.816	26.245	1.00 33.37
ATOM	2493	CB	THR	326	24.875	52.921	25.207	1.00 31.58
ATOM	2494	OG1	THR	326	24.934	53.617	23.956	1.00 29.82
ATOM	2495	CG2	THR	326	24.113	51.619	25.041	1.00 29.94
ATOM	2496	C	THR	326	23.951	53.016	27.515	1.00 33.05
ATOM	2497	O	THR	326	22.846	52.528	27.742	1.00 33.99
ATOM	2498	N	ARG	327	24.981	52.902	28.349	1.00 32.29
ATOM	2499	CA	ARG	327	24.859	52.148	29.588	1.00 31.76
ATOM	2500	CB	ARG	327	26.146	52.245	30.417	1.00 33.30
ATOM	2501	CG	ARG	327	26.226	51.162	31.485	1.00 36.71
ATOM	2502	CD	ARG	327	27.596	51.043	32.177	1.00 38.88
ATOM	2503	NE	ARG	327	27.795	52.024	33.249	1.00 40.62
ATOM	2504	CZ	ARG	327	28.274	53.255	33.069	1.00 41.13

Figure 4　　　　　　　　　　　　　　Sheet 45 of 62

ATOM	2505	NH1	ARG	327	28.615	53.670	31.846	1.00	40.49
ATOM	2506	NH2	ARG	327	28.393	54.078	34.113	1.00	40.82
ATOM	2507	C	ARG	327	23.681	52.691	30.387	1.00	30.62
ATOM	2508	O	ARG	327	22.888	51.930	30.940	1.00	29.96
ATOM	2509	N	PHE	328	23.559	54.014	30.425	1.00	29.60
ATOM	2510	CA	PHE	328	22.479	54.660	31.154	1.00	28.70
ATOM	2511	CB	PHE	328	22.632	56.176	31.069	1.00	28.03
ATOM	2512	CG	PHE	328	23.903	56.684	31.686	1.00	27.73
ATOM	2513	CD1	PHE	328	24.337	57.975	31.439	1.00	27.37
ATOM	2514	CD2	PHE	328	24.678	55.857	32.505	1.00	28.92
ATOM	2515	CE1	PHE	328	25.526	58.437	31.992	1.00	28.75
ATOM	2516	CE2	PHE	328	25.871	56.305	33.069	1.00	28.74
ATOM	2517	CZ	PHE	328	26.298	57.599	32.812	1.00	28.68
ATOM	2518	C	PHE	328	21.135	54.226	30.590	1.00	29.06
ATOM	2519	O	PHE	328	20.189	53.953	31.351	1.00	29.59
ATOM	2520	N	VAL	329	21.057	54.154	29.257	1.00	28.40
ATOM	2521	CA	VAL	329	19.830	53.735	28.587	1.00	26.44
ATOM	2522	CB	VAL	329	20.040	53.552	27.059	1.00	25.14
ATOM	2523	CG1	VAL	329	18.737	53.107	26.387	1.00	22.55
ATOM	2524	CG2	VAL	329	20.542	54.841	26.444	1.00	23.05
ATOM	2525	C	VAL	329	19.388	52.399	29.166	1.00	27.98
ATOM	2526	O	VAL	329	18.240	52.239	29.576	1.00	27.88
ATOM	2527	N	SER	330	20.308	51.442	29.219	1.00	28.76
ATOM	2528	CA	SER	330	19.966	50.117	29.718	1.00	30.08
ATOM	2529	CB	SER	330	21.136	49.171	29.534	1.00	30.45
ATOM	2530	OG	SER	330	20.720	47.852	29.822	1.00	31.92
ATOM	2531	C	SER	330	19.534	50.107	31.172	1.00	31.40
ATOM	2532	O	SER	330	18.690	49.298	31.577	1.00	31.74
ATOM	2533	N	GLN	331	20.118	50.993	31.972	1.00	32.45
ATOM	2534	CA	GLN	331	19.745	51.061	33.381	1.00	33.16
ATOM	2535	CB	GLN	331	20.668	51.992	34.151	1.00	33.58
ATOM	2536	CG	GLN	331	22.093	51.540	34.194	1.00	35.83
ATOM	2537	CD	GLN	331	22.947	52.534	34.919	1.00	37.72
ATOM	2538	OE1	GLN	331	22.626	52.927	36.043	1.00	39.62
ATOM	2539	NE2	GLN	331	24.042	52.958	34.291	1.00	38.98
ATOM	2540	C	GLN	331	18.327	51.591	33.482	1.00	33.78
ATOM	2541	O	GLN	331	17.428	50.881	33.938	1.00	34.06
ATOM	2542	N	VAL	332	18.129	52.835	33.038	1.00	33.77
ATOM	2543	CA	VAL	332	16.808	53.457	33.097	1.00	33.65
ATOM	2544	CB	VAL	332	16.760	54.791	32.282	1.00	32.19
ATOM	2545	CG1	VAL	332	17.279	54.584	30.905	1.00	33.04
ATOM	2546	CG2	VAL	332	15.340	55.312	32.215	1.00	31.67
ATOM	2547	C	VAL	332	15.695	52.505	32.638	1.00	34.20
ATOM	2548	O	VAL	332	14.571	52.566	33.139	1.00	34.51
ATOM	2549	N	GLU	333	16.001	51.607	31.711	1.00	34.30
ATOM	2550	CA	GLU	333	14.981	50.676	31.258	1.00	34.92
ATOM	2551	CB	GLU	333	15.210	50.289	29.795	1.00	34.40
ATOM	2552	CG	GLU	333	14.893	51.413	28.837	1.00	33.07
ATOM	2553	CD	GLU	333	14.806	50.956	27.409	1.00	31.80
ATOM	2554	OE1	GLU	333	13.983	50.060	27.114	1.00	31.65
ATOM	2555	OE2	GLU	333	15.561	51.504	26.581	1.00	31.72
ATOM	2556	C	GLU	333	14.949	49.438	32.135	1.00	35.76
ATOM	2557	O	GLU	333	14.163	48.520	31.911	1.00	35.73
ATOM	2558	N	SER	334	15.814	49.419	33.138	1.00	36.91
ATOM	2559	CA	SER	334	15.876	48.307	34.071	1.00	38.13
ATOM	2560	CB	SER	334	17.328	47.934	34.346	1.00	39.38
ATOM	2561	OG	SER	334	17.460	46.524	34.468	1.00	41.52

Figure 4   Sheet 46 of 62

```
ATOM   2562  C    SER   334      15.201  48.747  35.362  1.00  37.93
ATOM   2563  O    SER   334      15.053  47.973  36.306  1.00  38.63
ATOM   2564  N    ASP   335      14.807  50.014  35.385  1.00  38.51
ATOM   2565  CA   ASP   335      14.133  50.619  36.521  1.00  38.59
ATOM   2566  CB   ASP   335      13.776  52.061  36.173  1.00  39.10
ATOM   2567  CG   ASP   335      13.346  52.864  37.373  1.00  39.89
ATOM   2568  OD1  ASP   335      12.278  52.547  37.950  1.00  40.30
ATOM   2569  OD2  ASP   335      14.079  53.816  37.737  1.00  39.90
ATOM   2570  C    ASP   335      12.876  49.809  36.840  1.00  39.11
ATOM   2571  O    ASP   335      12.241  49.249  35.945  1.00  39.03
ATOM   2572  N    THR   336      12.517  49.768  38.119  1.00  39.68
ATOM   2573  CA   THR   336      11.372  48.999  38.605  1.00  39.94
ATOM   2574  CB   THR   336      11.773  48.297  39.896  1.00  39.68
ATOM   2575  OG1  THR   336      12.901  47.464  39.630  1.00  40.95
ATOM   2576  CG2  THR   336      10.650  47.452  40.426  1.00  39.84
ATOM   2577  C    THR   336      10.043  49.735  38.853  1.00  40.52
ATOM   2578  O    THR   336       8.984  49.108  38.931  1.00  40.91
ATOM   2579  N    GLY   337      10.085  51.054  38.970  1.00  40.80
ATOM   2580  CA   GLY   337       8.870  51.804  39.234  1.00  41.83
ATOM   2581  C    GLY   337       9.307  52.948  40.112  1.00  42.60
ATOM   2582  O    GLY   337       8.990  54.105  39.865  1.00  43.33
ATOM   2583  N    ASP   338      10.043  52.604  41.156  1.00  43.47
ATOM   2584  CA   ASP   338      10.606  53.589  42.059  1.00  44.40
ATOM   2585  CB   ASP   338      11.354  52.868  43.175  1.00  44.83
ATOM   2586  CG   ASP   338      12.303  51.808  42.637  1.00  45.34
ATOM   2587  OD1  ASP   338      11.879  51.032  41.751  1.00  46.12
ATOM   2588  OD2  ASP   338      13.465  51.742  43.087  1.00  45.59
ATOM   2589  C    ASP   338      11.597  54.296  41.142  1.00  44.84
ATOM   2590  O    ASP   338      12.605  53.709  40.756  1.00  45.53
ATOM   2591  N    ARG   339      11.310  55.533  40.763  1.00  44.81
ATOM   2592  CA   ARG   339      12.208  56.256  39.874  1.00  45.11
ATOM   2593  CB   ARG   339      11.702  57.687  39.654  1.00  45.72
ATOM   2594  CG   ARG   339      10.466  57.799  38.783  1.00  46.11
ATOM   2595  CD   ARG   339       9.201  57.413  39.521  1.00  46.99
ATOM   2596  NE   ARG   339       8.041  57.492  38.633  1.00  47.58
ATOM   2597  CZ   ARG   339       6.780  57.326  39.017  1.00  47.30
ATOM   2598  NH1  ARG   339       6.492  57.068  40.287  1.00  47.38
ATOM   2599  NH2  ARG   339       5.806  57.413  38.123  1.00  47.44
ATOM   2600  C    ARG   339      13.637  56.295  40.419  1.00  44.98
ATOM   2601  O    ARG   339      14.466  57.084  39.960  1.00  44.83
ATOM   2602  N    LYS   340      13.922  55.441  41.394  1.00  44.75
ATOM   2603  CA   LYS   340      15.238  55.394  42.001  1.00  45.05
ATOM   2604  CB   LYS   340      15.341  54.179  42.917  1.00  46.19
ATOM   2605  CG   LYS   340      14.358  54.250  44.081  1.00  47.87
ATOM   2606  CD   LYS   340      14.598  53.154  45.094  1.00  49.25
ATOM   2607  CE   LYS   340      13.365  52.949  45.957  1.00  50.44
ATOM   2608  NZ   LYS   340      13.353  51.589  46.598  1.00  51.78
ATOM   2609  C    LYS   340      16.398  55.422  41.014  1.00  44.66
ATOM   2610  O    LYS   340      17.186  56.372  41.026  1.00  44.90
ATOM   2611  N    GLN   341      16.509  54.408  40.155  1.00  43.94
ATOM   2612  CA   GLN   341      17.603  54.362  39.174  1.00  42.93
ATOM   2613  CB   GLN   341      17.598  53.028  38.435  1.00  45.04
ATOM   2614  CG   GLN   341      18.035  51.860  39.289  1.00  48.03
ATOM   2615  CD   GLN   341      18.758  50.801  38.482  1.00  49.69
ATOM   2616  OE1  GLN   341      19.731  51.101  37.779  1.00  50.67
ATOM   2617  NE2  GLN   341      18.297  49.556  38.581  1.00  50.43
ATOM   2618  C    GLN   341      17.616  55.497  38.146  1.00  40.93
```

```
ATOM   2619  O    GLN  341     18.672  56.057  37.839  1.00  38.85
ATOM   2620  N    ILE  342     16.449  55.824  37.600  1.00  39.61
ATOM   2621  CA   ILE  342     16.364  56.905  36.624  1.00  39.07
ATOM   2622  CB   ILE  342     14.920  57.110  36.130  1.00  39.24
ATOM   2623  CG2  ILE  342     14.880  58.226  35.107  1.00  39.19
ATOM   2624  CG1  ILE  342     14.392  55.817  35.501  1.00  39.87
ATOM   2625  CD1  ILE  342     12.945  55.902  35.070  1.00  40.76
ATOM   2626  C    ILE  342     16.832  58.185  37.301  1.00  38.43
ATOM   2627  O    ILE  342     17.704  58.892  36.795  1.00  37.48
ATOM   2628  N    TYR  343     16.240  58.466  38.456  1.00  38.93
ATOM   2629  CA   TYR  343     16.580  59.647  39.236  1.00  39.71
ATOM   2630  CB   TYR  343     15.813  59.656  40.567  1.00  40.97
ATOM   2631  CG   TYR  343     16.173  60.835  41.448  1.00  42.53
ATOM   2632  CD1  TYR  343     15.344  61.954  41.521  1.00  43.30
ATOM   2633  CE1  TYR  343     15.730  63.092  42.228  1.00  44.58
ATOM   2634  CD2  TYR  343     17.397  60.880  42.119  1.00  43.04
ATOM   2635  CE2  TYR  343     17.791  62.014  42.826  1.00  43.55
ATOM   2636  CZ   TYR  343     16.958  63.117  42.872  1.00  44.31
ATOM   2637  OH   TYR  343     17.369  64.260  43.523  1.00  45.74
ATOM   2638  C    TYR  343     18.070  59.635  39.532  1.00  39.93
ATOM   2639  O    TYR  343     18.789  60.598  39.262  1.00  40.28
ATOM   2640  N    ASN  344     18.525  58.529  40.098  1.00  40.14
ATOM   2641  CA   ASN  344     19.924  58.371  40.460  1.00  40.97
ATOM   2642  CB   ASN  344     20.146  56.958  40.989  1.00  42.94
ATOM   2643  CG   ASN  344     21.287  56.880  41.977  1.00  44.68
ATOM   2644  OD1  ASN  344     22.448  57.137  41.628  1.00  46.05
ATOM   2645  ND2  ASN  344     20.965  56.531  43.225  1.00  44.93
ATOM   2646  C    ASN  344     20.869  58.649  39.292  1.00  40.46
ATOM   2647  O    ASN  344     21.946  59.208  39.483  1.00  40.33
ATOM   2648  N    ILE  345     20.460  58.262  38.085  1.00  40.50
ATOM   2649  CA   ILE  345     21.280  58.467  36.890  1.00  39.89
ATOM   2650  CB   ILE  345     20.803  57.555  35.720  1.00  39.76
ATOM   2651  CG2  ILE  345     21.597  57.849  34.448  1.00  38.62
ATOM   2652  CG1  ILE  345     20.966  56.090  36.114  1.00  38.74
ATOM   2653  CD1  ILE  345     20.201  55.151  35.242  1.00  38.61
ATOM   2654  C    ILE  345     21.247  59.924  36.434  1.00  39.80
ATOM   2655  O    ILE  345     22.281  60.490  36.074  1.00  39.67
ATOM   2656  N    LEU  346     20.062  60.529  36.449  1.00  39.59
ATOM   2657  CA   LEU  346     19.912  61.923  36.029  1.00  39.58
ATOM   2658  CB   LEU  346     18.434  62.255  35.818  1.00  37.79
ATOM   2659  CG   LEU  346     17.809  61.528  34.625  1.00  36.58
ATOM   2660  CD1  LEU  346     16.277  61.599  34.684  1.00  35.18
ATOM   2661  CD2  LEU  346     18.363  62.145  33.337  1.00  35.05
ATOM   2662  C    LEU  346     20.519  62.892  37.034  1.00  40.82
ATOM   2663  O    LEU  346     21.177  63.857  36.654  1.00  41.02
ATOM   2664  N    SER  347     20.298  62.646  38.322  1.00  42.34
ATOM   2665  CA   SER  347     20.859  63.530  39.339  1.00  43.44
ATOM   2666  CB   SER  347     20.491  63.042  40.745  1.00  43.90
ATOM   2667  OG   SER  347     20.665  61.639  40.868  1.00  45.32
ATOM   2668  C    SER  347     22.368  63.556  39.156  1.00  43.44
ATOM   2669  O    SER  347     22.974  64.624  39.051  1.00  44.11
ATOM   2670  N    THR  348     22.969  62.374  39.096  1.00  43.10
ATOM   2671  CA   THR  348     24.407  62.285  38.909  1.00  42.97
ATOM   2672  CB   THR  348     24.853  60.830  38.700  1.00  42.31
ATOM   2673  OG1  THR  348     24.666  60.096  39.918  1.00  42.08
ATOM   2674  CG2  THR  348     26.322  60.780  38.282  1.00  40.85
ATOM   2675  C    THR  348     24.798  63.093  37.683  1.00  43.25
```

Figure 4   Sheet 48 of 62

```
ATOM   2676  O    THR   348      25.796  63.813  37.680  1.00  43.52
ATOM   2677  N    LEU   349      23.990  62.982  36.640  1.00  43.57
ATOM   2678  CA   LEU   349      24.271  63.697  35.412  1.00  44.17
ATOM   2679  CB   LEU   349      23.343  63.180  34.311  1.00  44.43
ATOM   2680  CG   LEU   349      23.787  63.204  32.847  1.00  44.86
ATOM   2681  CD1  LEU   349      25.198  62.658  32.688  1.00  44.59
ATOM   2682  CD2  LEU   349      22.790  62.375  32.046  1.00  44.64
ATOM   2683  C    LEU   349      24.102  65.201  35.638  1.00  44.32
ATOM   2684  O    LEU   349      24.317  66.003  34.726  1.00  45.33
ATOM   2685  N    GLY   350      23.722  65.574  36.862  1.00  43.94
ATOM   2686  CA   GLY   350      23.559  66.981  37.210  1.00  43.15
ATOM   2687  C    GLY   350      22.167  67.570  37.038  1.00  42.49
ATOM   2688  O    GLY   350      22.024  68.752  36.703  1.00  41.70
ATOM   2689  N    LEU   351      21.143  66.758  37.288  1.00  41.97
ATOM   2690  CA   LEU   351      19.758  67.197  37.132  1.00  41.45
ATOM   2691  CB   LEU   351      19.194  66.676  35.812  1.00  40.99
ATOM   2692  CG   LEU   351      19.875  67.115  34.522  1.00  40.66
ATOM   2693  CD1  LEU   351      19.516  66.144  33.416  1.00  41.63
ATOM   2694  CD2  LEU   351      19.453  68.533  34.172  1.00  40.77
ATOM   2695  C    LEU   351      18.858  66.718  38.262  1.00  41.15
ATOM   2696  O    LEU   351      19.170  65.760  38.973  1.00  40.88
ATOM   2697  N    ARG   352      17.720  67.379  38.410  1.00  41.10
ATOM   2698  CA   ARG   352      16.782  67.007  39.457  1.00  41.25
ATOM   2699  CB   ARG   352      16.614  68.173  40.431  1.00  42.65
ATOM   2700  CG   ARG   352      17.929  68.581  41.070  1.00  43.68
ATOM   2701  CD   ARG   352      18.504  67.421  41.851  1.00  45.59
ATOM   2702  NE   ARG   352      19.960  67.478  41.917  1.00  47.73
ATOM   2703  CZ   ARG   352      20.715  66.567  42.521  1.00  48.77
ATOM   2704  NH1  ARG   352      20.143  65.524  43.119  1.00  49.05
ATOM   2705  NH2  ARG   352      22.038  66.700  42.519  1.00  49.14
ATOM   2706  C    ARG   352      15.458  66.621  38.827  1.00  39.59
ATOM   2707  O    ARG   352      14.512  67.399  38.793  1.00  40.34
ATOM   2708  N    PRO   353      15.378  65.388  38.324  1.00  38.06
ATOM   2709  CD   PRO   353      16.325  64.285  38.555  1.00  37.28
ATOM   2710  CA   PRO   353      14.159  64.901  37.683  1.00  37.45
ATOM   2711  CB   PRO   353      14.595  63.552  37.134  1.00  37.27
ATOM   2712  CG   PRO   353      15.491  63.064  38.232  1.00  36.92
ATOM   2713  C    PRO   353      12.998  64.763  38.650  1.00  36.35
ATOM   2714  O    PRO   353      13.180  64.360  39.791  1.00  36.28
ATOM   2715  N    SER   354      11.805  65.110  38.194  1.00  35.82
ATOM   2716  CA   SER   354      10.625  64.951  39.028  1.00  36.40
ATOM   2717  CB   SER   354       9.570  66.010  38.698  1.00  35.94
ATOM   2718  OG   SER   354       8.944  65.725  37.459  1.00  35.63
ATOM   2719  C    SER   354      10.091  63.570  38.653  1.00  36.41
ATOM   2720  O    SER   354      10.592  62.948  37.716  1.00  37.42
ATOM   2721  N    THR   355       9.087  63.091  39.375  1.00  36.02
ATOM   2722  CA   THR   355       8.493  61.790  39.099  1.00  35.68
ATOM   2723  CB   THR   355       7.200  61.615  39.923  1.00  36.38
ATOM   2724  OG1  THR   355       7.525  61.645  41.316  1.00  37.75
ATOM   2725  CG2  THR   355       6.510  60.293  39.598  1.00  36.44
ATOM   2726  C    THR   355       8.161  61.633  37.609  1.00  35.80
ATOM   2727  O    THR   355       8.319  60.548  37.029  1.00  34.73
ATOM   2728  N    THR   356       7.698  62.720  36.994  1.00  35.28
ATOM   2729  CA   THR   356       7.336  62.690  35.586  1.00  35.39
ATOM   2730  CB   THR   356       6.287  63.774  35.263  1.00  35.59
ATOM   2731  OG1  THR   356       6.651  64.990  35.925  1.00  35.39
ATOM   2732  CG2  THR   356       4.892  63.331  35.719  1.00  34.33
```

Figure 4   Sheet 49 of 62

```
ATOM   2733  C    THR   356      8.542   62.848   34.662   1.00   35.30
ATOM   2734  O    THR   356      8.560   62.285   33.559   1.00   34.91
ATOM   2735  N    ASP   357      9.537   63.624   35.089   1.00   35.07
ATOM   2736  CA   ASP   357     10.740   63.782   34.277   1.00   35.80
ATOM   2737  CB   ASP   357     11.804   64.598   35.012   1.00   36.76
ATOM   2738  CG   ASP   357     11.451   66.077   35.116   1.00   38.19
ATOM   2739  OD1  ASP   357     11.475   66.778   34.071   1.00   37.60
ATOM   2740  OD2  ASP   357     11.158   66.538   36.249   1.00   38.76
ATOM   2741  C    ASP   357     11.277   62.373   34.039   1.00   35.97
ATOM   2742  O    ASP   357     11.460   61.942   32.901   1.00   36.94
ATOM   2743  N    CYS   358     11.498   61.649   35.131   1.00   35.67
ATOM   2744  CA   CYS   358     12.013   60.293   35.057   1.00   35.44
ATOM   2745  CB   CYS   358     12.051   59.658   36.447   1.00   35.93
ATOM   2746  SG   CYS   358     13.247   60.410   37.575   1.00   35.81
ATOM   2747  C    CYS   358     11.177   59.433   34.138   1.00   34.88
ATOM   2748  O    CYS   358     11.711   58.698   33.308   1.00   35.87
ATOM   2749  N    ASP   359      9.863   59.517   34.290   1.00   34.10
ATOM   2750  CA   ASP   359      8.960   58.729   33.464   1.00   33.10
ATOM   2751  CB   ASP   359      7.519   58.964   33.910   1.00   35.03
ATOM   2752  CG   ASP   359      7.118   58.058   35.062   1.00   36.65
ATOM   2753  OD1  ASP   359      7.950   57.850   35.975   1.00   38.15
ATOM   2754  OD2  ASP   359      5.969   57.561   35.055   1.00   37.12
ATOM   2755  C    ASP   359      9.130   59.058   31.985   1.00   31.16
ATOM   2756  O    ASP   359      9.090   58.170   31.133   1.00   30.01
ATOM   2757  N    ILE   360      9.325   60.334   31.682   1.00   29.54
ATOM   2758  CA   ILE   360      9.524   60.741   30.300   1.00   28.61
ATOM   2759  CB   ILE   360      9.546   62.273   30.162   1.00   27.75
ATOM   2760  CG2  ILE   360     10.255   62.668   28.874   1.00   27.01
ATOM   2761  CG1  ILE   360      8.112   62.818   30.235   1.00   26.18
ATOM   2762  CD1  ILE   360      8.024   64.322   30.190   1.00   23.23
ATOM   2763  C    ILE   360     10.857   60.176   29.825   1.00   29.21
ATOM   2764  O    ILE   360     10.919   59.480   28.805   1.00   29.88
ATOM   2765  N    VAL   361     11.923   60.466   30.569   1.00   28.39
ATOM   2766  CA   VAL   361     13.248   59.971   30.219   1.00   28.01
ATOM   2767  CB   VAL   361     14.258   60.256   31.342   1.00   27.73
ATOM   2768  CG1  VAL   361     15.575   59.551   31.055   1.00   27.43
ATOM   2769  CG2  VAL   361     14.492   61.759   31.453   1.00   27.76
ATOM   2770  C    VAL   361     13.245   58.464   29.919   1.00   27.74
ATOM   2771  O    VAL   361     14.055   57.982   29.107   1.00   27.40
ATOM   2772  N    ARG   362     12.341   57.719   30.556   1.00   27.72
ATOM   2773  CA   ARG   362     12.277   56.275   30.325   1.00   27.95
ATOM   2774  CB   ARG   362     11.523   55.571   31.455   1.00   29.48
ATOM   2775  CG   ARG   362     11.137   54.147   31.101   1.00   31.97
ATOM   2776  CD   ARG   362     10.900   53.266   32.308   1.00   33.93
ATOM   2777  NE   ARG   362     10.930   51.859   31.893   1.00   37.37
ATOM   2778  CZ   ARG   362     10.938   50.817   32.725   1.00   37.52
ATOM   2779  NH1  ARG   362     10.920   51.010   34.043   1.00   38.72
ATOM   2780  NH2  ARG   362     10.960   49.582   32.230   1.00   36.06
ATOM   2781  C    ARG   362     11.614   55.959   28.994   1.00   27.88
ATOM   2782  O    ARG   362     12.016   55.032   28.289   1.00   29.02
ATOM   2783  N    ARG   363     10.586   56.728   28.660   1.00   27.31
ATOM   2784  CA   ARG   363      9.866   56.564   27.400   1.00   25.77
ATOM   2785  CB   ARG   363      8.641   57.486   27.374   1.00   26.51
ATOM   2786  CG   ARG   363      7.530   57.084   28.318   1.00   26.30
ATOM   2787  CD   ARG   363      6.730   55.929   27.739   1.00   28.36
ATOM   2788  NE   ARG   363      6.259   56.216   26.380   1.00   30.91
ATOM   2789  CZ   ARG   363      6.872   55.826   25.260   1.00   31.55
```

Figure 4   Sheet 50 of 62

```
ATOM    2790  NH1 ARG    363       7.992  55.112  25.315  1.00  33.18   .
ATOM    2791  NH2 ARG    363       6.370  56.158  24.077  1.00  32.30
ATOM    2792  C   ARG    363      10.817  56.949  26.272  1.00  24.71
ATOM    2793  O   ARG    363      10.748  56.392  25.175  1.00  24.40
ATOM    2794  N   ALA    364      11.706  57.905  26.540  1.00  23.90
ATOM    2795  CA  ALA    364      12.653  58.339  25.507  1.00  24.48
ATOM    2796  CB  ALA    364      13.463  59.545  25.969  1.00  23.15
ATOM    2797  C   ALA    364      13.571  57.176  25.226  1.00  25.01
ATOM    2798  O   ALA    364      13.854  56.872  24.069  1.00  26.22
ATOM    2799  N   CYS    365      14.023  56.518  26.290  1.00  25.03
ATOM    2800  CA  CYS    365      14.902  55.370  26.157  1.00  24.77
ATOM    2801  CB  CYS    365      15.450  54.970  27.528  1.00  23.03
ATOM    2802  SG  CYS    365      16.728  56.114  28.173  1.00  21.60
ATOM    2803  C   CYS    365      14.140  54.206  25.514  1.00  26.44
ATOM    2804  O   CYS    365      14.661  53.535  24.617  1.00  27.49
ATOM    2805  N   GLU    366      12.906  53.956  25.944  1.00  26.87
ATOM    2806  CA  GLU    366      12.145  52.859  25.342  1.00  27.98
ATOM    2807  CB  GLU    366      10.757  52.743  25.988  1.00  28.74
ATOM    2808  CG  GLU    366      10.785  52.431  27.490  1.00  30.75
ATOM    2809  CD  GLU    366       9.427  51.981  28.041  1.00  32.09
ATOM    2810  OE1 GLU    366       8.444  52.757  27.970  1.00  32.39
ATOM    2811  OE2 GLU    366       9.342  50.841  28.547  1.00  33.30
ATOM    2812  C   GLU    366      12.005  53.056  23.815  1.00  28.15
ATOM    2813  O   GLU    366      12.117  52.104  23.029  1.00  27.63
ATOM    2814  N   SER    367      11.776  54.304  23.407  1.00  28.42
ATOM    2815  CA  SER    367      11.612  54.650  21.993  1.00  27.23
ATOM    2816  CB  SER    367      11.368  56.156  21.833  1.00  27.45
ATOM    2817  OG  SER    367      10.161  56.552  22.447  1.00  27.44
ATOM    2818  C   SER    367      12.824  54.276  21.165  1.00  26.52
ATOM    2819  O   SER    367      12.724  53.567  20.162  1.00  27.99
ATOM    2820  N   VAL    368      13.977  54.773  21.581  1.00  24.30
ATOM    2821  CA  VAL    368      15.194  54.499  20.849  1.00  22.45
ATOM    2822  CB  VAL    368      16.324  55.395  21.375  1.00  20.96
ATOM    2823  CG1 VAL    368      17.623  55.075  20.682  1.00  18.44
ATOM    2824  CG2 VAL    368      15.928  56.843  21.190  1.00  18.99
ATOM    2825  C   VAL    368      15.605  53.019  20.888  1.00  23.13
ATOM    2826  O   VAL    368      15.850  52.420  19.832  1.00  23.88
ATOM    2827  N   SER    369      15.660  52.405  22.071  1.00  22.54
ATOM    2828  CA  SER    369      16.071  51.003  22.106  1.00  21.93
ATOM    2829  CB  SER    369      16.248  50.476  23.542  1.00  23.39
ATOM    2830  OG  SER    369      15.011  50.251  24.197  1.00  25.91
ATOM    2831  C   SER    369      15.109  50.112  21.348  1.00  20.54
ATOM    2832  O   SER    369      15.526  49.063  20.850  1.00  20.31
ATOM    2833  N   THR    370      13.832  50.499  21.259  1.00  18.40
ATOM    2834  CA  THR    370      12.878  49.682  20.496  1.00  17.32
ATOM    2835  CB  THR    370      11.400  49.976  20.859  1.00  16.46
ATOM    2836  OG1 THR    370      11.053  49.298  22.073  1.00  15.81
ATOM    2837  CG2 THR    370      10.473  49.487  19.774  1.00  14.39
ATOM    2838  C   THR    370      13.076  49.936  19.001  1.00  17.03
ATOM    2839  O   THR    370      12.977  49.008  18.186  1.00  17.38
ATOM    2840  N   ARG    371      13.358  51.177  18.617  1.00  16.71
ATOM    2841  CA  ARG    371      13.562  51.423  17.201  1.00  16.54
ATOM    2842  CB  ARG    371      13.810  52.905  16.882  1.00  17.42
ATOM    2843  CG  ARG    371      14.013  53.123  15.374  1.00  17.76
ATOM    2844  CD  ARG    371      14.283  54.559  14.943  1.00  17.40
ATOM    2845  NE  ARG    371      15.567  55.076  15.412  1.00  18.85
ATOM    2846  CZ  ARG    371      16.159  56.154  14.896  1.00  18.99
```

Figure 4   Sheet 51 of 62

```
ATOM    2847  NH1 ARG   371      15.583  56.810  13.892  1.00  17.43
ATOM    2848  NH2 ARG   371      17.303  56.605  15.406  1.00  19.19
ATOM    2849  C   ARG   371      14.763  50.607  16.759  1.00  15.91
ATOM    2850  O   ARG   371      14.689  49.929  15.748  1.00  17.14
ATOM    2851  N   ALA   372      15.856  50.644  17.519  1.00  15.40
ATOM    2852  CA  ALA   372      17.061  49.883  17.148  1.00  16.23
ATOM    2853  CB  ALA   372      18.152  50.046  18.197  1.00  15.66
ATOM    2854  C   ALA   372      16.775  48.407  16.957  1.00  16.83
ATOM    2855  O   ALA   372      17.125  47.838  15.923  1.00  18.06
ATOM    2856  N   ALA   373      16.149  47.790  17.955  1.00  16.86
ATOM    2857  CA  ALA   373      15.817  46.367  17.912  1.00  17.10
ATOM    2858  CB  ALA   373      15.027  45.976  19.156  1.00  16.66
ATOM    2859  C   ALA   373      15.024  46.018  16.665  1.00  18.79
ATOM    2860  O   ALA   373      15.301  45.004  16.018  1.00  20.02
ATOM    2861  N   HIS   374      14.037  46.841  16.316  1.00  19.22
ATOM    2862  CA  HIS   374      13.243  46.560  15.122  1.00  20.89
ATOM    2863  CB  HIS   374      12.025  47.489  15.052  1.00  20.98
ATOM    2864  CG  HIS   374      10.948  47.131  16.029  1.00  19.79
ATOM    2865  CD2 HIS   374      10.813  46.065  16.855  1.00  19.53
ATOM    2866  ND1 HIS   374       9.833  47.914  16.229  1.00  19.92
ATOM    2867  CE1 HIS   374       9.057  47.347  17.137  1.00  18.78
ATOM    2868  NE2 HIS   374       9.629  46.223  17.532  1.00  18.61
ATOM    2869  C   HIS   374      14.075  46.696  13.866  1.00  21.57
ATOM    2870  O   HIS   374      14.136  45.789  13.058  1.00  21.42
ATOM    2871  N   MSE   375      14.722  47.835  13.698  1.00  24.00
ATOM    2872  CA  MSE   375      15.561  48.027  12.528  1.00  26.05
ATOM    2873  CB  MSE   375      16.390  49.311  12.666  1.00  28.31
ATOM    2874  CG  MSE   375      15.671  50.558  12.197  1.00  31.46
ATOM    2875  SE  MSE   375      15.246  50.448  10.400  1.00  41.26
ATOM    2876  CE  MSE   375      16.340  51.745   9.680  1.00  36.51
ATOM    2877  C   MSE   375      16.476  46.810  12.390  1.00  25.84
ATOM    2878  O   MSE   375      16.501  46.159  11.351  1.00  26.84
ATOM    2879  N   CYS   376      17.200  46.489  13.455  1.00  25.61
ATOM    2880  CA  CYS   376      18.107  45.349  13.436  1.00  25.11
ATOM    2881  CB  CYS   376      18.693  45.117  14.831  1.00  26.04
ATOM    2882  SG  CYS   376      20.038  43.879  14.876  1.00  27.98
ATOM    2883  C   CYS   376      17.445  44.058  12.931  1.00  24.01
ATOM    2884  O   CYS   376      18.015  43.369  12.078  1.00  24.35
ATOM    2885  N   SER   377      16.251  43.741  13.443  1.00  22.14
ATOM    2886  CA  SER   377      15.519  42.531  13.038  1.00  20.58
ATOM    2887  CB  SER   377      14.203  42.399  13.811  1.00  20.36
ATOM    2888  OG  SER   377      13.233  43.325  13.338  1.00  20.95
ATOM    2889  C   SER   377      15.210  42.535  11.542  1.00  20.00
ATOM    2890  O   SER   377      15.154  41.484  10.900  1.00  19.23
ATOM    2891  N   ALA   378      14.995  43.715  10.980  1.00  19.64
ATOM    2892  CA  ALA   378      14.723  43.787   9.549  1.00  19.32
ATOM    2893  CB  ALA   378      14.521  45.243   9.119  1.00  18.02
ATOM    2894  C   ALA   378      15.958  43.186   8.874  1.00  19.40
ATOM    2895  O   ALA   378      15.860  42.230   8.093  1.00  18.55
ATOM    2896  N   GLY   379      17.123  43.740   9.222  1.00  20.18
ATOM    2897  CA  GLY   379      18.381  43.271   8.669  1.00  20.06
ATOM    2898  C   GLY   379      18.547  41.762   8.734  1.00  19.52
ATOM    2899  O   GLY   379      18.754  41.113   7.704  1.00  20.07
ATOM    2900  N   LEU   380      18.442  41.201   9.936  1.00  18.61
ATOM    2901  CA  LEU   380      18.596  39.763  10.110  1.00  18.74
ATOM    2902  CB  LEU   380      18.489  39.371  11.579  1.00  18.49
ATOM    2903  CG  LEU   380      18.774  37.881  11.816  1.00  17.82
```

Figure 4   Sheet 52 of 62

```
ATOM    2904  CD1 LEU   380      20.215  37.586  11.383  1.00  16.94
ATOM    2905  CD2 LEU   380      18.557  37.512  13.285  1.00  16.34
ATOM    2906  C   LEU   380      17.580  38.938   9.341  1.00  19.56
ATOM    2907  O   LEU   380      17.895  37.833   8.892  1.00  20.67
ATOM    2908  N   ALA   381      16.354  39.447   9.211  1.00  19.83
ATOM    2909  CA  ALA   381      15.311  38.713   8.496  1.00  20.17
ATOM    2910  CB  ALA   381      13.961  39.327   8.759  1.00  19.87
ATOM    2911  C   ALA   381      15.638  38.746   7.009  1.00  21.06
ATOM    2912  O   ALA   381      15.421  37.773   6.269  1.00  21.05
ATOM    2913  N   GLY   382      16.174  39.874   6.567  1.00  21.33
ATOM    2914  CA  GLY   382      16.561  39.965   5.175  1.00  22.63
ATOM    2915  C   GLY   382      17.670  38.954   4.903  1.00  23.10
ATOM    2916  O   GLY   382      17.708  38.319   3.832  1.00  23.74
ATOM    2917  N   VAL   383      18.579  38.778   5.859  1.00  21.83
ATOM    2918  CA  VAL   383      19.642  37.828   5.615  1.00  22.47
ATOM    2919  CB  VAL   383      20.786  37.967   6.643  1.00  22.80
ATOM    2920  CG1 VAL   383      21.737  36.777   6.525  1.00  21.04
ATOM    2921  CG2 VAL   383      21.562  39.298   6.396  1.00  21.85
ATOM    2922  C   VAL   383      19.075  36.423   5.639  1.00  22.92
ATOM    2923  O   VAL   383      19.199  35.681   4.675  1.00  23.65
ATOM    2924  N   ILE   384      18.414  36.061   6.724  1.00  23.52
ATOM    2925  CA  ILE   384      17.853  34.721   6.835  1.00  24.64
ATOM    2926  CB  ILE   384      17.124  34.551   8.179  1.00  24.17
ATOM    2927  CG2 ILE   384      16.533  33.143   8.283  1.00  22.50
ATOM    2928  CG1 ILE   384      18.112  34.810   9.318  1.00  23.69
ATOM    2929  CD1 ILE   384      17.476  34.861  10.661  1.00  24.39
ATOM    2930  C   ILE   384      16.910  34.324   5.691  1.00  26.04
ATOM    2931  O   ILE   384      17.029  33.233   5.144  1.00  26.98
ATOM    2932  N   ASN   385      15.974  35.182   5.310  1.00  26.88
ATOM    2933  CA  ASN   385      15.097  34.785   4.218  1.00  27.99
ATOM    2934  CB  ASN   385      13.984  35.819   3.998  1.00  25.92
ATOM    2935  CG  ASN   385      13.038  35.918   5.174  1.00  23.68
ATOM    2936  OD1 ASN   385      12.721  34.921   5.820  1.00  21.60
ATOM    2937  ND2 ASN   385      12.567  37.128   5.448  1.00  23.03
ATOM    2938  C   ASN   385      15.888  34.579   2.915  1.00  29.62
ATOM    2939  O   ASN   385      15.610  33.647   2.143  1.00  29.62
ATOM    2940  N   ARG   386      16.869  35.440   2.660  1.00  31.30
ATOM    2941  CA  ARG   386      17.660  35.301   1.442  1.00  33.07
ATOM    2942  CB  ARG   386      18.840  36.261   1.446  1.00  32.62
ATOM    2943  CG  ARG   386      19.697  36.147   0.214  1.00  33.28
ATOM    2944  CD  ARG   386      20.908  37.059   0.284  1.00  34.52
ATOM    2945  NE  ARG   386      21.923  36.698  -0.704  1.00  35.29
ATOM    2946  CZ  ARG   386      21.812  36.910  -2.014  1.00  36.32
ATOM    2947  NH1 ARG   386      20.729  37.492  -2.518  1.00  35.95
ATOM    2948  NH2 ARG   386      22.782  36.525  -2.832  1.00  37.07
ATOM    2949  C   ARG   386      18.178  33.875   1.362  1.00  34.69
ATOM    2950  O   ARG   386      18.077  33.232   0.320  1.00  35.70
ATOM    2951  N   MSE   387      18.710  33.383   2.480  1.00  35.94
ATOM    2952  CA  MSE   387      19.250  32.036   2.560  1.00  37.39
ATOM    2953  CB  MSE   387      19.903  31.828   3.927  1.00  39.78
ATOM    2954  CG  MSE   387      21.099  32.754   4.186  1.00  42.37
ATOM    2955  SE  MSE   387      21.873  32.552   5.859  1.00  49.18
ATOM    2956  CE  MSE   387      21.738  30.694   6.097  1.00  44.67
ATOM    2957  C   MSE   387      18.179  30.976   2.311  1.00  38.50
ATOM    2958  O   MSE   387      18.463  29.927   1.721  1.00  37.80
ATOM    2959  N   ARG   388      16.954  31.255   2.769  1.00  40.15
ATOM    2960  CA  ARG   388      15.808  30.352   2.586  1.00  41.28
```

Figure 4 Sheet 53 of 62

```
ATOM   2961  CB   ARG   388     14.554  30.941   3.245  1.00  42.50
ATOM   2962  CG   ARG   388     13.268  30.115   3.069  1.00  42.73
ATOM   2963  CD   ARG   388     12.266  30.443   4.178  1.00  43.15
ATOM   2964  NE   ARG   388     10.965  29.787   4.012  1.00  44.47
ATOM   2965  CZ   ARG   388     10.049  30.134   3.104  1.00  44.46
ATOM   2966  NH1  ARG   388     10.283  31.139   2.269  1.00  44.11
ATOM   2967  NH2  ARG   388      8.895  29.478   3.033  1.00  44.15
ATOM   2968  C    ARG   388     15.579  30.210   1.094  1.00  41.39
ATOM   2969  O    ARG   388     15.516  29.104   0.554  1.00  40.76
ATOM   2970  N    GLU   389     15.460  31.355   0.439  1.00  41.88
ATOM   2971  CA   GLU   389     15.275  31.405  -0.997  1.00  43.37
ATOM   2972  CB   GLU   389     15.211  32.867  -1.448  1.00  45.21
ATOM   2973  CG   GLU   389     15.227  33.079  -2.957  1.00  48.22
ATOM   2974  CD   GLU   389     13.894  32.754  -3.632  1.00  50.35
ATOM   2975  OE1  GLU   389     13.850  32.799  -4.891  1.00  51.00
ATOM   2976  OE2  GLU   389     12.900  32.464  -2.912  1.00  50.86
ATOM   2977  C    GLU   389     16.476  30.713  -1.635  1.00  43.77
ATOM   2978  O    GLU   389     16.325  29.726  -2.355  1.00  43.53
ATOM   2979  N    SER   390     17.671  31.227  -1.335  1.00  43.84
ATOM   2980  CA   SER   390     18.925  30.697  -1.878  1.00  43.61
ATOM   2981  CB   SER   390     20.112  31.549  -1.425  1.00  43.41
ATOM   2982  OG   SER   390     20.229  32.703  -2.241  1.00  43.45
ATOM   2983  C    SER   390     19.243  29.234  -1.607  1.00  43.62
ATOM   2984  O    SER   390     20.126  28.671  -2.251  1.00  44.11
ATOM   2985  N    ARG   391     18.555  28.614  -0.660  1.00  43.22
ATOM   2986  CA   ARG   391     18.815  27.213  -0.396  1.00  43.67
ATOM   2987  CB   ARG   391     19.174  26.994   1.078  1.00  42.72
ATOM   2988  CG   ARG   391     20.440  27.699   1.512  1.00  41.51
ATOM   2989  CD   ARG   391     20.907  27.245   2.892  1.00  39.51
ATOM   2990  NE   ARG   391     22.183  27.864   3.231  1.00  37.99
ATOM   2991  CZ   ARG   391     22.940  27.512   4.266  1.00  37.81
ATOM   2992  NH1  ARG   391     22.545  26.540   5.070  1.00  36.05
ATOM   2993  NH2  ARG   391     24.105  28.121   4.482  1.00  37.12
ATOM   2994  C    ARG   391     17.578  26.404  -0.756  1.00  44.95
ATOM   2995  O    ARG   391     17.458  25.241  -0.372  1.00  45.05
ATOM   2996  N    SER   392     16.666  27.023  -1.502  1.00  46.71
ATOM   2997  CA   SER   392     15.420  26.367  -1.895  1.00  48.25
ATOM   2998  CB   SER   392     15.631  25.468  -3.121  1.00  48.10
ATOM   2999  OG   SER   392     15.610  26.216  -4.326  1.00  48.60
ATOM   3000  C    SER   392     14.880  25.536  -0.737  1.00  49.61
ATOM   3001  O    SER   392     14.601  24.344  -0.882  1.00  49.37
ATOM   3002  N    GLU   393     14.749  26.175   0.420  1.00  51.58
ATOM   3003  CA   GLU   393     14.237  25.510   1.617  1.00  53.54
ATOM   3004  CB   GLU   393     15.085  25.897   2.842  1.00  54.33
ATOM   3005  CG   GLU   393     16.586  25.655   2.701  1.00  54.92
ATOM   3006  CD   GLU   393     17.057  24.420   3.450  1.00  55.87
ATOM   3007  OE1  GLU   393     16.845  24.347   4.683  1.00  55.29
ATOM   3008  OE2  GLU   393     17.646  23.523   2.806  1.00  56.69
ATOM   3009  C    GLU   393     12.793  25.961   1.838  1.00  54.20
ATOM   3010  O    GLU   393     12.482  27.151   1.693  1.00  53.70
ATOM   3011  N    ASP   394     11.907  25.026   2.173  1.00  55.42
ATOM   3012  CA   ASP   394     10.519  25.404   2.419  1.00  56.88
ATOM   3013  CB   ASP   394      9.585  24.194   2.400  1.00  58.69
ATOM   3014  CG   ASP   394      8.111  24.602   2.415  1.00  61.23
ATOM   3015  OD1  ASP   394      7.691  25.298   3.376  1.00  62.29
ATOM   3016  OD2  ASP   394      7.374  24.237   1.466  1.00  62.03
ATOM   3017  C    ASP   394     10.489  26.041   3.795  1.00  56.57
```

Figure 4   Sheet 54 of 62

```
ATOM   3018  O    ASP   394    10.023  27.164   3.959  1.00  56.22
ATOM   3019  N    VAL   395    10.994  25.298   4.773  1.00  56.79
ATOM   3020  CA   VAL   395    11.086  25.756   6.153  1.00  57.23
ATOM   3021  CB   VAL   395    10.166  24.949   7.093  1.00  57.72
ATOM   3022  CG1  VAL   395    10.444  25.320   8.548  1.00  57.64
ATOM   3023  CG2  VAL   395     8.708  25.221   6.749  1.00  58.46
ATOM   3024  C    VAL   395    12.534  25.538   6.575  1.00  57.01
ATOM   3025  O    VAL   395    12.968  24.407   6.793  1.00  56.90
ATOM   3026  N    MSE   396    13.280  26.626   6.690  1.00  56.80
ATOM   3027  CA   MSE   396    14.682  26.536   7.058  1.00  56.12
ATOM   3028  CB   MSE   396    15.463  27.645   6.375  1.00  57.66
ATOM   3029  CG   MSE   396    16.932  27.623   6.690  1.00  60.51
ATOM   3030  SE   MSE   396    17.716  29.077   6.002  1.00  65.26
ATOM   3031  CE   MSE   396    17.988  28.564   4.293  1.00  64.74
ATOM   3032  C    MSE   396    14.964  26.600   8.545  1.00  54.59
ATOM   3033  O    MSE   396    14.487  27.491   9.245  1.00  54.08
ATOM   3034  N    ARG   397    15.740  25.637   9.025  1.00  53.05
ATOM   3035  CA   ARG   397    16.134  25.613  10.426  1.00  51.13
ATOM   3036  CB   ARG   397    16.226  24.181  10.951  1.00  52.77
ATOM   3037  CG   ARG   397    14.888  23.520  11.244  1.00  55.36
ATOM   3038  CD   ARG   397    15.132  22.079  11.671  1.00  58.69
ATOM   3039  NE   ARG   397    13.985  21.448  12.326  1.00  61.28
ATOM   3040  CZ   ARG   397    14.056  20.294  12.990  1.00  62.10
ATOM   3041  NH1  ARG   397    15.215  19.651  13.078  1.00  62.57
ATOM   3042  NH2  ARG   397    12.978  19.793  13.583  1.00  62.49
ATOM   3043  C    ARG   397    17.509  26.252  10.397  1.00  48.33
ATOM   3044  O    ARG   397    18.273  26.029   9.466  1.00  47.77
ATOM   3045  N    ILE   398    17.825  27.064  11.395  1.00  45.82
ATOM   3046  CA   ILE   398    19.120  27.721  11.396  1.00  43.01
ATOM   3047  CB   ILE   398    19.202  28.791  10.293  1.00  43.25
ATOM   3048  CG2  ILE   398    18.161  29.864  10.532  1.00  43.18
ATOM   3049  CG1  ILE   398    20.594  29.417  10.279  1.00  43.75
ATOM   3050  CD1  ILE   398    20.768  30.466   9.206  1.00  44.64
ATOM   3051  C    ILE   398    19.441  28.381  12.717  1.00  40.64
ATOM   3052  O    ILE   398    18.557  28.890  13.404  1.00  40.10
ATOM   3053  N    THR   399    20.722  28.360  13.060  1.00  37.78
ATOM   3054  CA   THR   399    21.185  28.954  14.290  1.00  35.36
ATOM   3055  CB   THR   399    22.052  27.988  15.079  1.00  35.02
ATOM   3056  OG1  THR   399    21.280  26.832  15.425  1.00  34.92
ATOM   3057  CG2  THR   399    22.570  28.666  16.345  1.00  34.73
ATOM   3058  C    THR   399    22.001  30.197  13.994  1.00  34.71
ATOM   3059  O    THR   399    22.736  30.254  13.005  1.00  35.10
ATOM   3060  N    VAL   400    21.858  31.184  14.871  1.00  32.96
ATOM   3061  CA   VAL   400    22.539  32.457  14.759  1.00  31.07
ATOM   3062  CB   VAL   400    21.514  33.593  14.592  1.00  31.21
ATOM   3063  CG1  VAL   400    22.211  34.934  14.415  1.00  31.76
ATOM   3064  CG2  VAL   400    20.628  33.298  13.405  1.00  31.47
ATOM   3065  C    VAL   400    23.336  32.685  16.039  1.00  30.19
ATOM   3066  O    VAL   400    22.779  32.640  17.144  1.00  30.96
ATOM   3067  N    GLY   401    24.641  32.905  15.888  1.00  28.35
ATOM   3068  CA   GLY   401    25.482  33.150  17.041  1.00  24.47
ATOM   3069  C    GLY   401    25.487  34.641  17.235  1.00  23.04
ATOM   3070  O    GLY   401    25.595  35.388  16.260  1.00  20.38
ATOM   3071  N    VAL   402    25.367  35.086  18.482  1.00  23.36
ATOM   3072  CA   VAL   402    25.338  36.514  18.751  1.00  23.38
ATOM   3073  CB   VAL   402    23.927  36.960  19.124  1.00  22.79
ATOM   3074  CG1  VAL   402    23.790  38.458  18.909  1.00  22.85
```

Figure 4   Sheet 55 of 62

```
ATOM  3075  CG2  VAL  402    22.895  36.176  18.320  1.00  22.42
ATOM  3076  C    VAL  402    26.252  36.899  19.893  1.00  24.25
ATOM  3077  O    VAL  402    26.484  36.098  20.794  1.00  25.20
ATOM  3078  N    ASP  403    26.770  38.124  19.848  1.00  24.83
ATOM  3079  CA   ASP  403    27.637  38.649  20.894  1.00  27.11
ATOM  3080  CB   ASP  403    29.078  38.212  20.691  1.00  30.98
ATOM  3081  CG   ASP  403    30.003  38.739  21.787  1.00  34.48
ATOM  3082  OD1  ASP  403    29.887  39.938  22.122  1.00  36.02
ATOM  3083  OD2  ASP  403    30.842  37.960  22.311  1.00  36.05
ATOM  3084  C    ASP  403    27.562  40.154  20.763  1.00  27.24
ATOM  3085  O    ASP  403    27.550  40.667  19.645  1.00  29.15
ATOM  3086  N    GLY  404    27.519  40.863  21.888  1.00  26.60
ATOM  3087  CA   GLY  404    27.410  42.316  21.863  1.00  26.50
ATOM  3088  C    GLY  404    26.750  42.829  23.137  1.00  27.10
ATOM  3089  O    GLY  404    25.810  42.193  23.665  1.00  26.90
ATOM  3090  N    SER  405    27.209  43.972  23.644  1.00  26.72
ATOM  3091  CA   SER  405    26.638  44.496  24.887  1.00  27.96
ATOM  3092  CB   SER  405    27.409  45.722  25.371  1.00  28.04
ATOM  3093  OG   SER  405    27.164  46.828  24.521  1.00  30.53
ATOM  3094  C    SER  405    25.168  44.857  24.738  1.00  28.25
ATOM  3095  O    SER  405    24.341  44.473  25.573  1.00  27.96
ATOM  3096  N    VAL  406    24.844  45.591  23.675  1.00  27.79
ATOM  3097  CA   VAL  406    23.465  45.992  23.445  1.00  28.13
ATOM  3098  CB   VAL  406    23.281  46.667  22.074  1.00  28.02
ATOM  3099  CG1  VAL  406    21.814  47.063  21.908  1.00  27.91
ATOM  3100  CG2  VAL  406    24.197  47.877  21.940  1.00  26.07
ATOM  3101  C    VAL  406    22.535  44.789  23.488  1.00  28.35
ATOM  3102  O    VAL  406    21.484  44.826  24.120  1.00  28.48
ATOM  3103  N    TYR  407    22.934  43.718  22.811  1.00  28.72
ATOM  3104  CA   TYR  407    22.130  42.493  22.736  1.00  28.45
ATOM  3105  CB   TYR  407    22.613  41.643  21.558  1.00  26.86
ATOM  3106  CG   TYR  407    21.831  40.373  21.341  1.00  25.29
ATOM  3107  CD1  TYR  407    20.700  40.358  20.535  1.00  25.44
ATOM  3108  CE1  TYR  407    19.964  39.189  20.346  1.00  25.93
ATOM  3109  CD2  TYR  407    22.213  39.192  21.955  1.00  24.93
ATOM  3110  CE2  TYR  407    21.488  38.021  21.780  1.00  25.18
ATOM  3111  CZ   TYR  407    20.362  38.024  20.974  1.00  26.03
ATOM  3112  OH   TYR  407    19.626  36.868  20.822  1.00  25.67
ATOM  3113  C    TYR  407    22.175  41.651  24.014  1.00  28.83
ATOM  3114  O    TYR  407    21.202  40.988  24.369  1.00  28.62
ATOM  3115  N    LYS  408    23.306  41.674  24.705  1.00  29.64
ATOM  3116  CA   LYS  408    23.440  40.881  25.916  1.00  30.07
ATOM  3117  CB   LYS  408    24.904  40.477  26.118  1.00  30.08
ATOM  3118  CG   LYS  408    25.442  39.556  25.030  1.00  30.61
ATOM  3119  CD   LYS  408    26.597  38.698  25.529  1.00  30.05
ATOM  3120  CE   LYS  408    26.799  37.515  24.601  1.00  30.22
ATOM  3121  NZ   LYS  408    27.828  36.573  25.097  1.00  30.20
ATOM  3122  C    LYS  408    22.940  41.551  27.185  1.00  30.82
ATOM  3123  O    LYS  408    22.327  40.901  28.038  1.00  31.98
ATOM  3124  N    LEU  409    23.176  42.853  27.296  1.00  30.97
ATOM  3125  CA   LEU  409    22.823  43.598  28.501  1.00  31.11
ATOM  3126  CB   LEU  409    24.006  44.482  28.875  1.00  30.54
ATOM  3127  CG   LEU  409    25.305  43.700  28.962  1.00  29.31
ATOM  3128  CD1  LEU  409    26.372  44.591  29.597  1.00  29.41
ATOM  3129  CD2  LEU  409    25.067  42.423  29.785  1.00  28.16
ATOM  3130  C    LEU  409    21.548  44.441  28.611  1.00  31.44
ATOM  3131  O    LEU  409    20.978  44.542  29.708  1.00  31.86
```

Figure 4 Sheet 56 of 62

```
ATOM   3132  N   HIS  410      21.122  45.077  27.519  1.00  31.34
ATOM   3133  CA  HIS  410      19.929  45.912  27.572  1.00  30.80
ATOM   3134  CB  HIS  410      19.732  46.635  26.247  1.00  30.36
ATOM   3135  CG  HIS  410      18.703  47.717  26.303  1.00  29.89
ATOM   3136  CD2 HIS  410      18.815  49.060  26.179  1.00  29.29
ATOM   3137  ND1 HIS  410      17.362  47.457  26.508  1.00  30.79
ATOM   3138  CE1 HIS  410      16.691  48.595  26.505  1.00  29.88
ATOM   3139  NE2 HIS  410      17.548  49.583  26.309  1.00  30.87
ATOM   3140  C   HIS  410      18.728  45.031  27.900  1.00  31.41
ATOM   3141  O   HIS  410      18.467  44.055  27.207  1.00  31.97
ATOM   3142  N   PRO  411      17.985  45.376  28.969  1.00  31.63
ATOM   3143  CD  PRO  411      18.173  46.690  29.610  1.00  31.32
ATOM   3144  CA  PRO  411      16.798  44.708  29.518  1.00  31.33
ATOM   3145  CB  PRO  411      16.111  45.815  30.299  1.00  31.27
ATOM   3146  CG  PRO  411      17.257  46.599  30.822  1.00  32.32
ATOM   3147  C   PRO  411      15.827  44.037  28.571  1.00  32.09
ATOM   3148  O   PRO  411      15.362  42.920  28.838  1.00  32.76
ATOM   3149  N   SER  412      15.519  44.684  27.457  1.00  31.73
ATOM   3150  CA  SER  412      14.527  44.094  26.573  1.00  31.92
ATOM   3151  CB  SER  412      13.210  44.834  26.771  1.00  32.51
ATOM   3152  OG  SER  412      13.368  46.200  26.390  1.00  33.27
ATOM   3153  C   SER  412      14.838  44.047  25.082  1.00  31.91
ATOM   3154  O   SER  412      14.039  43.520  24.304  1.00  32.59
ATOM   3155  N   PHE  413      15.974  44.601  24.679  1.00  30.72
ATOM   3156  CA  PHE  413      16.348  44.615  23.271  1.00  30.13
ATOM   3157  CB  PHE  413      17.778  45.105  23.130  1.00  28.18
ATOM   3158  CG  PHE  413      18.213  45.285  21.716  1.00  25.96
ATOM   3159  CD1 PHE  413      18.085  46.522  21.094  1.00  25.70
ATOM   3160  CD2 PHE  413      18.772  44.233  21.015  1.00  24.47
ATOM   3161  CE1 PHE  413      18.517  46.711  19.787  1.00  25.13
ATOM   3162  CE2 PHE  413      19.208  44.408  19.707  1.00  24.84
ATOM   3163  CZ  PHE  413      19.082  45.652  19.092  1.00  24.48
ATOM   3164  C   PHE  413      16.232  43.228  22.645  1.00  31.20
ATOM   3165  O   PHE  413      15.571  43.026  21.612  1.00  31.56
ATOM   3166  N   LYS  414      16.888  42.268  23.275  1.00  31.75
ATOM   3167  CA  LYS  414      16.851  40.906  22.790  1.00  32.75
ATOM   3168  CB  LYS  414      17.626  39.999  23.755  1.00  33.66
ATOM   3169  CG  LYS  414      17.570  38.526  23.429  1.00  34.45
ATOM   3170  CD  LYS  414      18.732  37.744  24.049  1.00  36.05
ATOM   3171  CE  LYS  414      18.845  37.909  25.558  1.00  35.80
ATOM   3172  NZ  LYS  414      19.972  38.817  25.920  1.00  36.66
ATOM   3173  C   LYS  414      15.412  40.411  22.600  1.00  33.19
ATOM   3174  O   LYS  414      15.054  39.927  21.518  1.00  33.30
ATOM   3175  N   GLU  415      14.577  40.542  23.627  1.00  33.81
ATOM   3176  CA  GLU  415      13.193  40.071  23.513  1.00  34.53
ATOM   3177  CB  GLU  415      12.462  40.251  24.838  1.00  37.66
ATOM   3178  CG  GLU  415      13.062  39.497  26.002  1.00  42.83
ATOM   3179  CD  GLU  415      14.376  40.090  26.520  1.00  45.68
ATOM   3180  OE1 GLU  415      14.523  41.339  26.526  1.00  47.31
ATOM   3181  OE2 GLU  415      15.245  39.293  26.956  1.00  47.44
ATOM   3182  C   GLU  415      12.409  40.776  22.401  1.00  33.23
ATOM   3183  O   GLU  415      11.676  40.137  21.649  1.00  33.06
ATOM   3184  N   ARG  416      12.551  42.092  22.299  1.00  31.77
ATOM   3185  CA  ARG  416      11.841  42.825  21.264  1.00  30.32
ATOM   3186  CB  ARG  416      12.066  44.328  21.427  1.00  31.27
ATOM   3187  CG  ARG  416      11.645  44.875  22.796  1.00  33.92
ATOM   3188  CD  ARG  416      11.783  46.393  22.901  1.00  35.48
```

Figure 4   Sheet 57 of 62

```
ATOM    3189  NE   ARG   416    11.545  46.866  24.267  1.00  38.24
ATOM    3190  CZ   ARG   416    11.982  48.030  24.746  1.00  39.11
ATOM    3191  NH1  ARG   416    12.676  48.850  23.967  1.00  39.89
ATOM    3192  NH2  ARG   416    11.754  48.365  26.009  1.00  38.52
ATOM    3193  C    ARG   416    12.379  42.354  19.916  1.00  29.08
ATOM    3194  O    ARG   416    11.620  42.159  18.964  1.00  28.85
ATOM    3195  N    PHE   417    13.694  42.144  19.862  1.00  27.59
ATOM    3196  CA   PHE   417    14.377  41.707  18.648  1.00  25.70
ATOM    3197  CB   PHE   417    15.886  41.687  18.890  1.00  23.64
ATOM    3198  CG   PHE   417    16.687  41.310  17.680  1.00  20.59
ATOM    3199  CD1  PHE   417    16.910  42.230  16.671  1.00  18.99
ATOM    3200  CD2  PHE   417    17.183  40.018  17.540  1.00  19.41
ATOM    3201  CE1  PHE   417    17.610  41.870  15.540  1.00  19.87
ATOM    3202  CE2  PHE   417    17.884  39.641  16.413  1.00  18.04
ATOM    3203  CZ   PHE   417    18.100  40.563  15.409  1.00  20.04
ATOM    3204  C    PHE   417    13.943  40.342  18.099  1.00  25.74
ATOM    3205  O    PHE   417    13.568  40.225  16.927  1.00  25.24
ATOM    3206  N    HIS   418    14.012  39.301  18.922  1.00  26.11
ATOM    3207  CA   HIS   418    13.612  37.962  18.459  1.00  26.79
ATOM    3208  CB   HIS   418    13.638  36.973  19.615  1.00  28.01
ATOM    3209  CG   HIS   418    14.973  36.854  20.279  1.00  28.81
ATOM    3210  CD2  HIS   418    16.168  37.425  19.989  1.00  29.42
ATOM    3211  ND1  HIS   418    15.182  36.067  21.389  1.00  28.15
ATOM    3212  CE1  HIS   418    16.446  36.157  21.755  1.00  29.43
ATOM    3213  NE2  HIS   418    17.067  36.974  20.924  1.00  29.74
ATOM    3214  C    HIS   418    12.209  37.985  17.876  1.00  26.41
ATOM    3215  O    HIS   418    11.976  37.565  16.733  1.00  26.40
ATOM    3216  N    ALA   419    11.284  38.487  18.688  1.00  25.83
ATOM    3217  CA   ALA   419     9.885  38.603  18.328  1.00  25.05
ATOM    3218  CB   ALA   419     9.182  39.454  19.352  1.00  24.80
ATOM    3219  C    ALA   419     9.731  39.215  16.943  1.00  25.35
ATOM    3220  O    ALA   419     9.146  38.601  16.029  1.00  25.99
ATOM    3221  N    SER   420    10.249  40.425  16.777  1.00  25.26
ATOM    3222  CA   SER   420    10.159  41.078  15.481  1.00  25.31
ATOM    3223  CB   SER   420    10.897  42.405  15.515  1.00  23.85
ATOM    3224  OG   SER   420    10.692  43.089  14.303  1.00  23.43
ATOM    3225  C    SER   420    10.751  40.170  14.391  1.00  26.14
ATOM    3226  O    SER   420    10.145  39.976  13.331  1.00  25.95
ATOM    3227  N    VAL   421    11.926  39.602  14.670  1.00  27.34
ATOM    3228  CA   VAL   421    12.602  38.699  13.733  1.00  28.41
ATOM    3229  CB   VAL   421    13.919  38.127  14.346  1.00  27.63
ATOM    3230  CG1  VAL   421    14.479  37.020  13.475  1.00  26.36
ATOM    3231  CG2  VAL   421    14.953  39.232  14.469  1.00  28.22
ATOM    3232  C    VAL   421    11.689  37.535  13.325  1.00  29.65
ATOM    3233  O    VAL   421    11.557  37.227  12.130  1.00  28.72
ATOM    3234  N    ARG   422    11.069  36.886  14.310  1.00  30.74
ATOM    3235  CA   ARG   422    10.165  35.775  14.014  1.00  32.79
ATOM    3236  CB   ARG   422     9.419  35.328  15.265  1.00  33.29
ATOM    3237  CG   ARG   422    10.259  35.197  16.512  1.00  34.47
ATOM    3238  CD   ARG   422    11.081  33.927  16.558  1.00  34.54
ATOM    3239  NE   ARG   422    11.862  33.905  17.795  1.00  35.75
ATOM    3240  CZ   ARG   422    12.824  33.028  18.066  1.00  35.45
ATOM    3241  NH1  ARG   422    13.127  32.085  17.180  1.00  35.35
ATOM    3242  NH2  ARG   422    13.490  33.108  19.215  1.00  33.55
ATOM    3243  C    ARG   422     9.123  36.277  13.019  1.00  33.41
ATOM    3244  O    ARG   422     8.949  35.728  11.929  1.00  33.68
ATOM    3245  N    ARG   423     8.446  37.348  13.417  1.00  34.00
```

Figure 4   Sheet 58 of 62

ATOM	3246	CA	ARG	423	7.394	37.946	12.622	1.00	34.13
ATOM	3247	CB	ARG	423	7.022	39.301	13.207	1.00	35.16
ATOM	3248	CG	ARG	423	5.538	39.584	13.202	1.00	36.10
ATOM	3249	CD	ARG	423	5.212	40.831	14.012	1.00	37.57
ATOM	3250	NE	ARG	423	5.482	40.682	15.441	1.00	38.90
ATOM	3251	CZ	ARG	423	6.274	41.503	16.133	1.00	40.51
ATOM	3252	NH1	ARG	423	6.874	42.523	15.513	1.00	41.42
ATOM	3253	NH2	ARG	423	6.461	41.324	17.440	1.00	38.76
ATOM	3254	C	ARG	423	7.754	38.100	11.165	1.00	33.94
ATOM	3255	O	ARG	423	6.919	37.849	10.295	1.00	35.59
ATOM	3256	N	LEU	424	8.993	38.494	10.884	1.00	32.85
ATOM	3257	CA	LEU	424	9.418	38.699	9.497	1.00	31.57
ATOM	3258	CB	LEU	424	10.474	39.788	9.450	1.00	28.75
ATOM	3259	CG	-LEU	424	10.030	41.129	10.003	1.00	27.64
ATOM	3260	CD1	LEU	424	11.220	42.080	10.066	1.00	26.47
ATOM	3261	CD2	LEU	424	8.942	41.686	9.115	1.00	27.23
ATOM	3262	C	LEU	424	9.950	37.479	8.747	1.00	32.00
ATOM	3263	O	LEU	424	10.232	37.562	7.551	1.00	31.15
ATOM	3264	N	THR	425	10.065	36.343	9.424	1.00	33.88
ATOM	3265	CA	THR	425	10.615	35.153	8.778	1.00	35.30
ATOM	3266	CB	THR	425	11.886	34.722	9.495	1.00	35.17
ATOM	3267	OG1	THR	425	11.580	34.463	10.874	1.00	35.24
ATOM	3268	CG2	THR	425	12.939	35.817	9.399	1.00	35.16
ATOM	3269	C	THR	425	9.711	33.923	8.675	1.00	37.00
ATOM	3270	O	THR	425	10.059	32.854	9.182	1.00	37.54
ATOM	3271	N	PRO	426	8.562	34.040	7.982	1.00	38.04
ATOM	3272	CD	PRO	426	8.144	35.123	7.073	1.00	38.49
ATOM	3273	CA	PRO	426	7.663	32.890	7.856	1.00	38.85
ATOM	3274	CB	PRO	426	6.745	33.295	6.700	1.00	38.23
ATOM	3275	CG	PRO	426	6.699	34.772	6.802	1.00	38.07
ATOM	3276	C	PRO	426	8.445	31.615	7.527	1.00	39.83
ATOM	3277	O	PRO	426	9.378	31.641	6.728	1.00	40.28
ATOM	3278	N	SER	427	8.073	30.510	8.158	1.00	40.72
ATOM	3279	CA	SER	427	8.713	29.232	7.892	1.00	41.82
ATOM	3280	CB	SER	427	8.358	28.785	6.474	1.00	42.86
ATOM	3281	OG	SER	427	6.954	28.802	6.287	1.00	44.69
ATOM	3282	C	SER	427	10.234	29.228	8.068	1.00	42.10
ATOM	3283	O	SER	427	10.981	28.899	7.140	1.00	41.85
ATOM	3284	N	CYS	428	10.679	29.586	9.267	1.00	42.60
ATOM	3285	CA	CYS	428	12.096	29.608	9.601	1.00	42.43
ATOM	3286	CB	CYS	428	12.724	30.960	9.258	1.00	42.59
ATOM	3287	SG	CYS	428	12.860	31.327	7.492	1.00	44.02
ATOM	3288	C	CYS	428	12.195	29.381	11.096	1.00	42.45
ATOM	3289	O	CYS	428	11.671	30.169	11.879	1.00	43.76
ATOM	3290	N	GLU	429	12.846	28.296	11.494	1.00	42.34
ATOM	3291	CA	GLU	429	13.014	27.995	12.909	1.00	41.23
ATOM	3292	CB	GLU	429	13.030	26.486	13.146	1.00	42.97
ATOM	3293	CG	GLU	429	11.699	25.796	12.933	1.00	45.48
ATOM	3294	CD	GLU	429	11.847	24.282	12.925	1.00	47.43
ATOM	3295	OE1	GLU	429	12.518	23.756	13.847	1.00	48.77
ATOM	3296	OE2	GLU	429	11.298	23.623	12.005	1.00	48.07
ATOM	3297	C	GLU	429	14.341	28.587	13.346	1.00	39.77
ATOM	3298	O	GLU	429	15.370	27.902	13.352	1.00	39.92
ATOM	3299	N	ILE	430	14.315	29.864	13.708	1.00	38.09
ATOM	3300	CA	ILE	430	15.514	30.560	14.142	1.00	36.48
ATOM	3301	CB	ILE	430	15.341	32.070	13.998	1.00	35.17
ATOM	3302	CG2	ILE	430	16.659	32.770	14.280	1.00	34.48

```
ATOM   3303  CG1  ILE   430     14.839  32.390  12.589  1.00  35.30
ATOM   3304  CD1  ILE   430     14.669  33.866  12.310  1.00  34.88
ATOM   3305  C    ILE   430     15.872  30.254  15.591  1.00  37.06
ATOM   3306  O    ILE   430     15.044  30.399  16.495  1.00  38.13
ATOM   3307  N    THR   431     17.109  29.823  15.808  1.00  36.61
ATOM   3308  CA   THR   431     17.600  29.520  17.146  1.00  36.17
ATOM   3309  CB   THR   431     18.067  28.053  17.240  1.00  36.58
ATOM   3310  OG1  THR   431     16.950  27.180  17.031  1.00  36.34
ATOM   3311  CG2  THR   431     18.692  27.774  18.604  1.00  36.38
ATOM   3312  C    THR   431     18.796  30.441  17.396  1.00  36.13
ATOM   3313  O    THR   431     19.705  30.513  16.569  1.00  36.10
ATOM   3314  N    PHE   432     18.804  31.157  18.514  1.00  35.79
ATOM   3315  CA   PHE   432     19.926  32.054  18.794  1.00  35.93
ATOM   3316  CB   PHE   432     19.443  33.450  19.232  1.00  34.31
ATOM   3317  CG   PHE   432     18.643  34.194  18.188  1.00  32.53
ATOM   3318  CD1  PHE   432     17.271  33.977  18.048  1.00  31.59
ATOM   3319  CD2  PHE   432     19.262  35.124  17.353  1.00  31.00
ATOM   3320  CE1  PHE   432     16.527  34.676  17.092  1.00  30.53
ATOM   3321  CE2  PHE   432     18.525  35.826  16.395  1.00  30.25
ATOM   3322  CZ   PHE   432     17.154  35.600  16.266  1.00  30.11
ATOM   3323  C    PHE   432     20.767  31.483  19.917  1.00  37.08
ATOM   3324  O    PHE   432     20.248  30.772  20.779  1.00  38.85
ATOM   3325  N    ILE   433     22.063  31.774  19.906  1.00  37.32
ATOM   3326  CA   ILE   433     22.933  31.321  20.983  1.00  38.46
ATOM   3327  CB   ILE   433     23.526  29.890  20.722  1.00  39.06
ATOM   3328  CG2  ILE   433     22.398  28.863  20.624  1.00  38.62
ATOM   3329  CG1  ILE   433     24.367  29.861  19.449  1.00  39.03
ATOM   3330  CD1  ILE   433     25.028  28.520  19.227  1.00  38.32
ATOM   3331  C    ILE   433     24.039  32.358  21.161  1.00  39.33
ATOM   3332  O    ILE   433     24.429  33.034  20.201  1.00  39.15
ATOM   3333  N    GLU   434     24.527  32.505  22.388  1.00  40.58
ATOM   3334  CA   GLU   434     25.559  33.498  22.669  1.00  42.92
ATOM   3335  CB   GLU   434     25.152  34.312  23.885  1.00  43.91
ATOM   3336  CG   GLU   434     23.769  34.883  23.744  1.00  45.53
ATOM   3337  CD   GLU   434     23.342  35.640  24.965  1.00  46.68
ATOM   3338  OE1  GLU   434     23.436  35.072  26.074  1.00  47.18
ATOM   3339  OE2  GLU   434     22.910  36.802  24.816  1.00  48.77
ATOM   3340  C    GLU   434     26.965  32.950  22.865  1.00  44.01
ATOM   3341  O    GLU   434     27.206  32.058  23.680  1.00  44.48
ATOM   3342  N    SER   435     27.901  33.518  22.119  1.00  45.00
ATOM   3343  CA   SER   435     29.284  33.075  22.167  1.00  46.11
ATOM   3344  CB   SER   435     30.077  33.779  21.057  1.00  46.95
ATOM   3345  OG   SER   435     29.839  35.186  21.053  1.00  47.94
ATOM   3346  C    SER   435     29.984  33.274  23.507  1.00  46.36
ATOM   3347  O    SER   435     30.043  34.396  24.022  1.00  46.31
ATOM   3348  N    GLU   436     30.505  32.180  24.069  1.00  46.22
ATOM   3349  CA   GLU   436     31.248  32.250  25.330  1.00  46.33
ATOM   3350  CB   GLU   436     31.322  30.884  26.020  1.00  47.64
ATOM   3351  CG   GLU   436     32.144  30.908  27.317  1.00  50.83
ATOM   3352  CD   GLU   436     32.726  29.541  27.711  1.00  52.03
ATOM   3353  OE1  GLU   436     31.951  28.585  27.970  1.00  52.84
ATOM   3354  OE2  GLU   436     33.972  29.428  27.765  1.00  52.07
ATOM   3355  C    GLU   436     32.650  32.671  24.912  1.00  45.58
ATOM   3356  O    GLU   436     33.446  31.843  24.463  1.00  45.50
ATOM   3357  N    GLU   437     32.950  33.956  25.051  1.00  44.67
ATOM   3358  CA   GLU   437     34.252  34.462  24.643  1.00  44.13
ATOM   3359  CB   GLU   437     35.328  34.050  25.652  1.00  43.61
```

Figure 4   Sheet 60 of 62

```
ATOM   3360  CG  GLU   437     36.745  34.334  25.190  1.00  43.39
ATOM   3361  CD  GLU   437     36.931  35.752  24.678  1.00  43.50
ATOM   3362  OE1 GLU   437     36.976  36.680  25.514  1.00  44.49
ATOM   3363  OE2 GLU   437     37.025  35.940  23.441  1.00  42.17
ATOM   3364  C   GLU   437     34.569  33.880  23.264  1.00  43.56
ATOM   3365  O   GLU   437     35.530  33.131  23.108  1.00  45.30
ATOM   3366  N   GLY   438     33.757  34.225  22.266  1.00  41.68
ATOM   3367  CA  GLY   438     33.958  33.700  20.926  1.00  39.44
ATOM   3368  C   GLY   438     34.748  34.538  19.934  1.00  38.11
ATOM   3369  O   GLY   438     34.932  34.130  18.791  1.00  37.45
ATOM   3370  N   SER   439     35.213  35.713  20.329  1.00  37.14
ATOM   3371  CA  SER   439     35.980  36.502  19.386  1.00  36.86
ATOM   3372  CB  SER   439     35.916  37.983  19.714  1.00  36.81
ATOM   3373  OG  SER   439     36.825  38.678  18.878  1.00  35.32
ATOM   3374  C   SER   439     37.420  36.053  19.444  1.00  36.74
ATOM   3375  O   SER   439     38.192  36.265  18.513  1.00  36.37
ATOM   3376  N   GLY   440     37.774  35.439  20.562  1.00  36.58
ATOM   3377  CA  GLY   440     39.126  34.957  20.746  1.00  36.42
ATOM   3378  C   GLY   440     39.207  33.518  20.302  1.00  36.28
ATOM   3379  O   GLY   440     40.146  33.140  19.613  1.00  36.20
ATOM   3380  N   ARG   441     38.224  32.714  20.699  1.00  36.09
ATOM   3381  CA  ARG   441     38.190  31.309  20.312  1.00  37.16
ATOM   3382  CB  ARG   441     37.151  30.562  21.138  1.00  37.34
ATOM   3383  CG  ARG   441     37.312  30.717  22.632  1.00  39.57
ATOM   3384  CD  ARG   441     36.334  29.806  23.375  1.00  42.28
ATOM   3385  NE  ARG   441     35.270  29.339  22.488  1.00  44.36
ATOM   3386  CZ  ARG   441     34.240  28.585  22.862  1.00  45.80
ATOM   3387  NH1 ARG   441     34.103  28.192  24.127  1.00  45.87
ATOM   3388  NH2 ARG   441     33.346  28.214  21.955  1.00  47.26
ATOM   3389  C   ARG   441     37.848  31.179  18.821  1.00  37.42
ATOM   3390  O   ARG   441     38.103  30.151  18.189  1.00  37.52
ATOM   3391  N   GLY   442     37.270  32.234  18.262  1.00  37.34
ATOM   3392  CA  GLY   442     36.906  32.204  16.863  1.00  37.39
ATOM   3393  C   GLY   442     38.165  32.308  16.048  1.00  37.47
ATOM   3394  O   GLY   442     38.483  31.410  15.278  1.00  37.51
ATOM   3395  N   ALA   443     38.887  33.408  16.241  1.00  38.17
ATOM   3396  CA  ALA   443     40.134  33.660  15.526  1.00  38.50
ATOM   3397  CB  ALA   443     40.739  34.999  15.967  1.00  36.50
ATOM   3398  C   ALA   443     41.127  32.521  15.759  1.00  39.03
ATOM   3399  O   ALA   443     42.015  32.297  14.941  1.00  39.36
ATOM   3400  N   ALA   444     40.977  31.807  16.875  1.00  39.93
ATOM   3401  CA  ALA   444     41.864  30.685  17.172  1.00  40.31
ATOM   3402  CB  ALA   444     41.724  30.242  18.623  1.00  39.25
ATOM   3403  C   ALA   444     41.427  29.569  16.246  1.00  40.97
ATOM   3404  O   ALA   444     42.146  29.210  15.312  1.00  41.31
ATOM   3405  N   LEU   445     40.233  29.038  16.501  1.00  41.41
ATOM   3406  CA  LEU   445     39.678  27.960  15.690  1.00  41.97
ATOM   3407  CB  LEU   445     38.195  27.776  16.024  1.00  40.09
ATOM   3408  CG  LEU   445     37.954  26.806  17.182  1.00  39.14
ATOM   3409  CD1 LEU   445     36.750  27.233  17.982  1.00  39.27
ATOM   3410  CD2 LEU   445     37.781  25.399  16.647  1.00  37.36
ATOM   3411  C   LEU   445     39.860  28.156  14.176  1.00  43.29
ATOM   3412  O   LEU   445     39.918  27.179  13.427  1.00  43.28
ATOM   3413  N   VAL   446     39.955  29.406  13.729  1.00  44.66
ATOM   3414  CA  VAL   446     40.136  29.684  12.307  1.00  46.32
ATOM   3415  CB  VAL   446     39.687  31.120  11.948  1.00  46.15
ATOM   3416  CG1 VAL   446     40.356  31.578  10.653  1.00  46.15
```

Figure 4   Sheet 61 of 62

```
ATOM   3417   CG2  VAL   446    38.164  31.160  11.793  1.00  45.75
ATOM   3418   C    VAL   446    41.597  29.503  11.944  1.00  48.03
ATOM   3419   O    VAL   446    41.929  29.105  10.825  1.00  48.75
ATOM   3420   N    SER   447    42.465  29.802  12.904  1.00  49.63
ATOM   3421   CA   SER   447    43.902  29.657  12.725  1.00  50.76
ATOM   3422   CB   SER   447    44.635  30.267  13.918  1.00  50.76
ATOM   3423   OG   SER   447    44.377  31.659  14.021  1.00  50.83
ATOM   3424   C    SER   447    44.259  28.173  12.612  1.00  52.07
ATOM   3425   O    SER   447    44.923  27.753  11.662  1.00  52.17
ATOM   3426   N    ALA   448    43.804  27.387  13.584  1.00  53.51
ATOM   3427   CA   ALA   448    44.071  25.953  13.621  1.00  55.46
ATOM   3428   CB   ALA   448    43.273  25.306  14.745  1.00  55.02
ATOM   3429   C    ALA   448    43.751  25.263  12.300  1.00  57.02
ATOM   3430   O    ALA   448    44.599  24.564  11.726  1.00  57.18
ATOM   3431   N    VAL   449    42.523  25.457  11.825  1.00  58.39
ATOM   3432   CA   VAL   449    42.093  24.841  10.579  1.00  59.69
ATOM   3433   CB   VAL   449    40.571  24.977  10.382  1.00  59.67
ATOM   3434   CG1  VAL   449    40.152  24.262   9.112  1.00  60.28
ATOM   3435   CG2  VAL   449    39.833  24.384  11.577  1.00  59.48
ATOM   3436   C    VAL   449    42.821  25.482   9.403  1.00  60.70
ATOM   3437   O    VAL   449    42.903  24.898   8.321  1.00  61.00
ATOM   3438   N    ALA   450    43.361  26.677   9.627  1.00  61.41
ATOM   3439   CA   ALA   450    44.093  27.392   8.591  1.00  62.12
ATOM   3440   CB   ALA   450    43.981  28.889   8.814  1.00  62.32
ATOM   3441   C    ALA   450    45.558  26.973   8.606  1.00  63.02
ATOM   3442   O    ALA   450    46.437  27.748   8.217  1.00  62.75
ATOM   3443   N    CYS   451    45.807  25.744   9.061  1.00  64.03
ATOM   3444   CA   CYS   451    47.160  25.183   9.148  1.00  65.19
ATOM   3445   CB   CYS   451    47.530  24.440   7.850  1.00  65.75
ATOM   3446   SG   CYS   451    46.901  22.720   7.723  1.00  66.86
ATOM   3447   C    CYS   451    48.239  26.217   9.474  1.00  65.22
ATOM   3448   O    CYS   451    47.929  27.230  10.144  1.00  65.18
ATOM   3449   OXT  CYS   451    49.398  25.979   9.073  1.00  65.50
ATOM   3450   C1   HEX     1    31.023  47.521  12.611  1.00  25.83
ATOM   3451   C2   HEX     1    32.239  47.182  11.801  1.00  25.25
ATOM   3452   C3   HEX     1    32.203  45.697  11.565  1.00  25.11
ATOM   3453   C4   HEX     1    32.071  44.939  12.862  1.00  24.99
ATOM   3454   C5   HEX     1    31.030  45.591  13.785  1.00  25.34
ATOM   3455   C6   HEX     1    30.772  44.921  15.126  1.00  25.58
ATOM   3456   O1   HEX     1    30.750  48.942  12.579  1.00  27.04
ATOM   3457   O2   HEX     1    32.183  47.912  10.609  1.00  24.71
ATOM   3458   O3   HEX     1    33.337  45.251  10.836  1.00  25.99
ATOM   3459   O4   HEX     1    31.699  43.621  12.545  1.00  25.85
ATOM   3460   O5   HEX     1    31.267  46.968  13.935  1.00  25.37
ATOM   3461   O6   HEX     1    31.835  45.222  16.009  1.00  27.23
ATOM   3462   C1   LIG     1    30.034  26.620   8.669  1.00  35.87
ATOM   3463   C2   LIG     1    29.909  27.259  10.064  1.00  34.82
ATOM   3464   C3   LIG     1    31.308  27.852  10.344  1.00  35.54
ATOM   3465   C4   LIG     1    32.212  27.447   9.148  1.00  35.52
ATOM   3466   C5   LIG     1    31.520  26.207   8.584  1.00  35.20
ATOM   3467   C6   LIG     1    33.670  27.245   9.637  1.00  36.33
ATOM   3468   C7   LIG     1    34.562  26.321   8.758  1.00  37.11
ATOM   3469   C8   LIG     1    35.946  26.832   8.778  1.00  36.91
ATOM   3470   N9   LIG     1    36.382  27.317   7.570  1.00  36.92
ATOM   3471   C10  LIG     1    37.668  27.907   7.331  1.00  36.42
ATOM   3472   N11  LIG     1    38.035  28.336   6.087  1.00  37.39
ATOM   3473   C12  LIG     1    39.058  28.930   6.462  1.00  36.99
```

Figure 4   Sheet 62 of 62

```
ATOM   3474   C13  LIG      1      39.426  29.003   7.575  1.00 37.10
ATOM   3475   S14  LIG      1      38.681  28.342   8.700  1.00 37.86
ATOM   3476   O15  LIG      1      36.640  26.843   9.817  1.00 38.32
ATOM   3477   C16  LIG      1      34.538  24.890   9.296  1.00 37.59
ATOM   3478   C17  LIG      1      34.906  24.620  10.610  1.00 37.22
ATOM   3479   C18  LIG      1      34.658  23.346  11.130  1.00 38.09
ATOM   3480   N19  LIG      1      34.084  22.371  10.404  1.00 38.80
ATOM   3481   C20  LIG      1      33.729  22.598   9.128  1.00 38.90
ATOM   3482   C21  LIG      1      33.942  23.860   8.546  1.00 38.73
ATOM   3483   K1   K        1      32.471  32.037  -7.104  1.00 46.91
END
```